

Fakultät für Elektrotechnik, Informatik und Mathematik

#### Coherent light backscattering phenomena of powder-like surfaces

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## Kurzfassung

In dieser Arbeit wird die Streuung von Licht an pulverförmigen Oberflächen betrachtet und hat dabei einen Fokus auf der kohärenten Doppelstreuung, die eine negative Polarisation und einen Intensitätsanstieg bei der Rückstreuung erzeugt. Die beiden Effekte werden Oppositionsphänomene genannt. Das für eine theoretische Analyse zu lösende elektrodynamische Problem wird numerisch mithilfe des diskontinuierlichen Galerkin-Verfahrens im Zeitbereich auf Hochleistungsrechnern gelöst. Simuliert wird dabei die Streuung von unpolarisiertem Licht an den Strukturen, die aus eng angeordneten Teilchen bestehen. Dazu gehören binäre Kugeln, Würfel, unregelmäßige Teilchen und dicht gepackte Schichten aus bis zu zehn unregelmäßigen Teilchen. Diese bestehen aus absorbierendem Material und sind dabei viel größer als die Wellenlänge des einfallenden Lichts. Simulationen zeigen, dass die Strukturen einiger weniger unregelmäßiger Teilchen in der Lage sind, den negativen Polarisationseffekt zu klären, der bei natürlichen, pulverartigen Oberflächen und Laborproben beobachtet wird. Simulationen für regelmäßige Formen mit kontrollierten Geometrien wie Würfel, facettierte Kugeln und Ellipsoide liefern aufschlussreiche Erklärungen, welche Rolle die Geometrie und Packungsdichte des Streusystems für die Oppositionsphänomene spielen. Sie zeigen, dass der Interferenz-Mechanismus empfindlich auf die Geometrie der Streuer reagiert und nicht nur zu einer negativen Polarisation, sondern auch zu einer Verstärkung der positiven Polarisation oder sogar zu keiner Polarisation bei der Rückstreuung führen kann. Selbst zwei zufällig orientierte unregelmäßige Teilchen zeigen eine schwache negative Polarisation. Im Gegensatz dazu erzeugen einzelne absorbierende Teilchen keine Polarisation, was den zuvor vorgeschlagenen Mechanismus der Doppelstreuung bestätigt. Wenn man der Struktur mehr Teilchen hinzufügt, erhöht sich der relative Beitrag der Doppelstreuung, was die negative Polarisation bei der Rückstreuung verstärkt. Numerische Berechnungen zeigen keine direkte Korrelation zwischen negativer Polarisation und Intensitätsanstieg. Eine Abflachung der Teilchengeometrien in Lichteinfallsrichtung in einer Schicht kann die negative Polarisation verringern oder sogar aufheben. Gleichzeitig erhöht sich die Intensität bei der Rückstreuung aufgrund des höheren Beitrags der Streuung von einem einzelnen Teilchen.

### Abstract

In this work, the scattering of light from powder-like surfaces is considered with focus on coherent double scattering mechanism, which produces negative polarization and an intensity surge at backscattering. Both effects are called *opposition phenomena*. To analyze them theoretically, a full-wave electrodynamic problem is solved numerically using the discontinuous Galerkin time domain method (DGTD) and high performance computing. Unpolarized light scattering from structures consisting of closely positioned particles is simulated. These include binary spheres, cubes, random irregular particles and densely packed layers of up to ten irregular particles. The particles consist of absorbing material and have sizes much larger than the wavelength of incident light. Simulations show that the structures of a few irregular particles are able to the reproduce negative polarization effect, that is observed for natural powder-like surfaces and laboratory samples. Simulations for regular shapes with controlled geometries such as cubes, faceted spheres and ellipsoids provided insightful explanation of the role played by geometry and packing density of the scattering system on the opposition phenomena. They indicate that the interference mechanism is sensitive to the geometry of the scatterers and can result not only in negative polarization, but also, in enhancement of the positive polarization or even no polarization at backscattering. Even two randomly oriented irregular particles show a weak negative polarization. In contrast, single absorbing particles do not produce it, which confirms double scattering mechanism suggested previously. Adding more particles to the structure increases the relative contribution of double-scattering, which enhances negative polarization near backscattering. Numerical computations did not confirm a direct correlation between negative polarization and intensity surge. Flattening of particle geometries in the direction of incident light in a layer can reduce or even eliminate the negative polarization. At the same time, this increases the intensity at backscattering due to dominance of single scattering.

## **Publications**

The work on this thesis was accompanied by the following publications:

- 1. Samer Alhaddad, Yevgen Grynko, Henna Farheen, and Jens Förstner. Numerical analysis of the coherent mechanism producing negative polarization at backscattering from systems of absorbing particles. *Optics letters*, 47(1):58–61, 2022. [113]
- 2. Samer Alhaddad, Jens Förstner, Stefan Groth, Daniel Grünewald, Yevgen Grynko, Frank Hannig, Tobias Kenter, F.J. Pfreundt, Christian Plessl, Merlind Schotte, Thomas Steinke, J. Teich, Martin Weiser, and Florian Wende. The highpermeshes framework for numerical algorithms on unstructured grids. *Concurrency and Computation: Practice and Experience*, page e6616, 2021. [117]
- Samer Alhaddad, Jens Förstner, Stefan Groth, Daniel Grünewald, Yevgen Grynko, Frank Hannig, Tobias Kenter, Franz-Josef Pfreundt, Christian Plessl, Merlind Schotte, et al. Highpermeshes-a domain-specific language for numerical algorithms on unstructured grids. In *European Conference on Parallel Processing*, pages 185–196. Springer, 2020. [74]
- Yevgen Grynko, Yuriy Shkuratov, Samer Alhaddad, and Jens Förstner. Light scattering by large densely packed clusters of particles. In Springer Series in Light Scattering. Springer, 2022, accepted. [114]
- 5. Yevgen Grynko, Yuriy Shkuratov, Samer Alhaddad, and Jens Förstner. Negative polarization of light at backscattering from a numerical analog of planetary regoliths. *Icarus*, 2022, submitted. [115]
- Manfred Hammer, Lena Ebers, Andre Hildebrandt, Samer Alhaddad, and Jens Förstner. Oblique semi-guided waves: 2-d integrated photonics with negative effective permittivity. In 2018 IEEE 17th International Conference on Mathematical Methods in Electromagnetic Theory (MMET), pages 9–15. IEEE, 2018. [40]

- Tobias Kenter, Gopinath Mahale, Samer Alhaddad, Yevgen Grynko, Christian Schmitt, Ayesha Afzal, Frank Hannig, Jens Förstner, and Christian Plessl. Openclbased fpga design to accelerate the nodal discontinuous galerkin method for unstructured meshes. In 2018 IEEE 26th Annual International Symposium on Field-Programmable Custom Computing Machines (FCCM), pages 189–196. IEEE, 2018. [75]
- Ayesha Afzal, Christian Schmitt, Samer Alhaddad, Yevgen Grynko, Jurgen Teich, Jens Forstner, and Frank Hannig. Solving maxwell's equations with modern c++ and sycl: A case study. In 2018 IEEE 29th International Conference on Applicationspecific Systems, Architectures and Processors (ASAP), pages 1–8. IEEE, 2018. [76]
- Manfred Hammer, Samer Alhaddad, and Jens Förstner. Hybrid coupled-mode modeling in 3d: perturbed and coupled channels, and waveguide crossings. JOSA B, 34(3):613–624, 2017. [41]
- Andre Hildebrandt, Samer Alhaddad, Manfred Hammer, and Jens Förstner. Oblique incidence of semi-guided waves on step-like folds in planar dielectric slabs: Lossless vertical interconnects in 3d integrated photonic circuits. In *Integrated Optics: Devices, Materials, and Technologies XX*, volume 9750, pages 249–255. SPIE, 2016. [42]

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## Introduction

Light scattered by the objects in nature is first of all this, what we perceive with our eyes to recognize our surroundings, characterize and explore the environment around us. Very simply, without it we can not see.

This work focuses on light scattered from discrete objects or particles and powderlike surfaces. In general, light scattering in discrete random media has been studied and analyzed in different scientific areas like optics and photonics [1–3], biology and medicine [4–8] and astronomy for planetary regoliths and Solar System bodies [9–14], cosmic dust [15, 16] and optical remote sensing of Earth [17, 18]. The goal of this thesis is solving the light scattering problem for optical remote sensing applications with a numerical method. Planetary regoliths are composed of randomly oriented, densely packed and irregularly shaped particles. Optical measurements are used here to get Stokes parameters of light scattered from different objects to study their scattering properties. Polarimetric and photometric observations of light scattered by these particles deliver information about the physical properties and geometric topologies of the scattering system [9, 12, 13, 19-21]. This information can be derived from intensity and polarization characteristics. The intensity and polarization can be represented as functions of the scattering angles. At this point it is worthy to define the scattering angle  $\theta$  (see figures 1.2 and 1.3) as the angle constructed between the direction of the incoming electromagnetic wave to the direction of observation. In some literature the phase angle  $\alpha$  is used instead of the scattering one. There is only one difference between them that the phase angle takes the opposite direction of the incoming wave into account instead of the forward one  $(\alpha = \pi - \theta)$ . An example of a real photopolarimetric observation from the Moon is shown in figure 1.1. The curves are plotted with the phase angle  $\alpha$ . The plots in figure 1.1 show negative polarization and intensity surge obtained near and at the backscattering direction.



Figure 1.1: Phase angle curves of (a) normalized intensity and (b) linear polarization of the Moon. The plots are taken from Fig. 3. in the reference [22].



Figure 1.2: Light scattered from single uniquely shaped particle. The scattering angle  $\theta$  is between the positive z-direction and the scattering one ( $\theta \in [0^\circ, 180^\circ]$ ).

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Figure 1.3: Light scattered from monolayer of ten uniquely shaped particles. The scattering angle  $\theta$  is between the positive z-direction and the scattering one ( $\theta \in [0^{\circ}, 180^{\circ}]$ ).

The linear polarization is described by  $P = (I_{\perp} - I_{\parallel})/(I_{\perp} + I_{\parallel})$ , where  $I_{\parallel}$  and  $I_{\perp}$  are intensities measured in different perpendicular planes. Both effects are common in remote sensing observations and laboratory measurements [23]. They are called opposition or backscattering phenomena and demonstrated in figures 1.4 and 1.5, respectively. Negative polarization and intensity surge can correlate with each other under some conditions and sometimes they do not show remarkable relationship between them [9].

The intensity and polarization of any scattering system can be retrieved from its scattering matrix (if it is known), which in general, describes the system answer to electromagnetic waves illumination. This scattering matrix is gained from the Stokes parameters [24, 25] regarding to the incident and scattered light, which in turn, is calculated by solving Maxwell equations [24]. Particles sizes [26–28], particles size distribution and packing density [29], real and complex refractive index [30] and surface roughness [31–33] can affect the light scattering behavior of the studied system for all directions or some of them in different ways. As example, some affected characteristics here at backscattering are the amplitude of negative polarization, the existence and grade of the intensity surge, as well as the correlation between intensity surge and negative polarization and the inversion angle where the polarization turn over from the positive side to the negative one [9].



Figure 1.4: Typical scattering angle dependency of the linear polarization degree with approximate classification of scattering regions (forward, intermediate and backscattering).



Figure 1.5: Typical scattering angle dependency of the normalized intensity with approximate classification of scattering regions (forward, intermediate and backscattering).

#### CHAPTER 1. INTRODUCTION

In order to consider the problem of light scattering from a system, a model that can be studied theoretically is needed. Analytical solutions are restricted to simple or well known geometries. An analytical solution for agglomerates of randomly distributed irregular particles does not exist. This is due to the diverse packing density, large scale complex geometry and material composition of the scattering objects. What adds more complexity to the scattering problem is the near field interaction between the closely neighbored particles, which involve further decisive contribution to the scattered field. Therefore, in order to analyze the observational photopolarimetric data and for solving the inverse problem, a clear understanding of the mechanisms that are responsible for the formation of negative polarization and the intensity surge is essential. This work contributes to explaining the origin of the negative polarization, gives clarification of the existence of both intensity surge and negative polarization and systematically examines the correlation between them.

Considering the powders regarding to their refractive index, and correspondingly, their material, gives two categorizations of high and low absorbing particles and low and high albedo, respectively. Figure 1.6 displays an example of a regolith sample returned by a space mission from the asteroid Ryugy that has low albedo (0.044 to 0.050) [34,35].



Figure 1.6: low albedo regolith sample returned from the asteroid Ryugu by the space mission Hayabusa2. The picture is adopted from reference [34].

For low or non-absorbing constituents the negative polarization obviously arises from single scattering by particles lying on the surface [29], where increasing the packing density enhances the negative polarization because of reducing the multiple scattering contribution. However, having high absorbing materials, which is the focus of this work, also reduces the multiple scattering in such way that just the first few orders of scattering are involved and can influence the opposition effects. The negative polarization and the intensity surge are observed in laboratory measurements for absorbing powders (e.g. [26]). The negative polarization here seems to be produced by the double and not the single scattering. This is demonstrated by approximate double scattering models that take into consideration point scatterers with different single scattering features, for example Fresnel scatterers [36, 37], random distribution of electric dipoles [38] or small particles with Rayleigh polarization phase functions [39].

A theoretical modeling of light scattering from powder-like structures, that mimic the behavior of real powders, can provide reasonable answers and explanations for the opposition phenomena. Controlling parameters of the model (like density, geometry, surface roughness, orientation and refractive index of the particles) can deliver analyzable results that support solving this complex problem. As currently there is no available analytical solution for this, it can be only treated with numerical modeling. In many scientific and industrial applications the numerical simulations become increasingly important and help to understand the underlying mechanisms of physical systems, predict system behavior, engineer interesting geometries [40–42], design processes and optimize systems without dealing with fabrication procedures and finally solve inverse problems. Furthermore, when studying the dynamics of a physical system, its partial differential equations (PDEs), which describe its behavior mathematically, need to be solved in space and time.

Generally, there are two categorizations for numerical methods: Approximate and numerically exact ones. For instance, Geometrical Optics approximation (GO) that belongs to the first classification [43–47] is simple and fast. It does not consider wave effects that can not be ignored for investigating the origin of the negative polarization, especially, when the particles have the same scale of the wavelength of incident light. It is used for studying light scattering by large particles. However, it has been improved for single scattering by ice crystals in order to get approximated solutions close to the ones obtained by exact numerical methods [48].

Solving the problem with full-wave exact numerical methods without approximations gives more trustworthy results and in-depth conceptual clarification of the light backscattering phenomena. A widely used one for electrodynamic computations in general is the finite difference time domain method (FDTD) [49–51]. Here, the simulation domain gets tessellated to get a structured grid. Such grids are not spatially flexible, especially, for irregular or curvilinear geometries like the shapes considered in this work. A popular numerical approach in the light scattering community is the Discrete Dipole Approximation method (DDA) [52–54]. It has been developed to study light scattered from irregular particles. Its principle bases on discretizing the illuminated object into small cubical or non-cubical volumes (small dipoles). Then the electric field volume integral equation in these scatterers is numerically solved [52]. There are available parallelized codes as open source for DDA [55]. Nevertheless, the relative accuracy and computational performance of DDA decrease for larger refractive indices of materials. As well, with increasing

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scatterer size, the computing time steeply grows. [53, 56]. The DDA method is also sensitive to the resolution of the discretized small scatterers and their chosen shape. Thus, discretization and shape errors can appear [52].

Also, the T-matrix method is widely used for light scattering computations [57]. Originally, it is suitable for dense clusters of spherical particles or sparse agglomerates of irregular ones. Results gained by T-matrix approach for complex structured particles have agreement with laboratory measurements [58]. However, this is not always the case due to uncertainty in its numerical approach and the approximations of such realistic models, as it is explained in the same paper. There are T-matrix method codes that deal with electromagnetic scattering from nonspherical randomly oriented particles that are rotationally symmetric and homogeneous [59]. There are also other parallel open source public codes that can be run on high performance computing (HPC) platforms (e.g. [60, 61]). In spite of that, this method becomes complicated if a scatterer has no rotational symmetry and has random shape. Additionally, for some scattering objects with large sizes, edges or surface roughness, T-matrix method becomes numerically unstable [62]. Large packing density for irregular particles is also hardly possible. However, it has been extended to simulate pairs of ellipsoids that lie in close neighborhood [63].

In this work, light scattering problems for different structures of particles of different shapes with absorbing material are solved numerically to study the mechanisms responsible for opposition phenomena. The Discontinuous Galerkin method in time domain (DGTD) is applied [64–67]. This is a full-wave numerical approach allowing spatial flexibility as it is a variant of finite element method (FEM) [68, 69]. Importantly, it can be parallelized to run on high performance computers due to its compact numerical scheme and local mathematical operations for each mesh element of the discretized simulation domain. When dealing with large scale problems for powder structures having complex geometry as a real model an efficient parallel code, that runs on HPC platforms is needed. The used software is an in-house code based on the numerical scheme of Hesthaven and Warburton [65] with further additional implementations by Grynko and Foerstner [66].

Studying the scattering from a single particle can help for understanding the scattering by a constitution of particles. However, the goal of this thesis is studying the optical opposition phenomena of systems consisting of absorbing, closely packed, irregular particles that have sizes larger than the wavelength of the incident light, which is the case for a lot of natural powders [24]. Additionally, simulations for regular shapes such as cubes, faceted spheres and ellipsoids are done to investigate the influence of geometry on opposition phenomena.

# 2

## Theoretical basis of light scattering

Light scattering simulation is an electrodynamic problem, in which Maxwell's equations are solved. These are partial differential equations (PDEs) that describe the behavior of the electromagnetic waves in space ( $\mathbf{r} \begin{bmatrix} m \end{bmatrix}$  is the space vector) over time  $t \begin{bmatrix} s \end{bmatrix}$ . They couple the electric  $\mathbf{E} \begin{bmatrix} \frac{V}{m} \end{bmatrix}$  and the magnetic  $\mathbf{H} \begin{bmatrix} \frac{A}{m} \end{bmatrix}$  fields with the magnetic and the electric inductions  $\mathbf{B} \begin{bmatrix} \frac{Vs}{m^2} \end{bmatrix}$ ,  $\mathbf{D} \begin{bmatrix} \frac{C}{m^2} \end{bmatrix}$ , respectively [24,70,71]. The macroscopic Maxwell's equations are given as follows:

$$\operatorname{rot} \mathbf{E}(\mathbf{r}, t) = -\dot{\mathbf{B}}(\mathbf{r}, t)$$
  

$$\operatorname{rot} \mathbf{H}(\mathbf{r}, t) = \dot{\mathbf{D}}(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t)$$
  

$$\operatorname{div} \mathbf{D}(\mathbf{r}, t) = \rho(\mathbf{r}, t)$$
  

$$\operatorname{div} \mathbf{B}(\mathbf{r}, t) = 0$$
(2.1)

The vectors and matrices in this work are denoted with bold mathematical symbols. The point over  $\dot{\mathbf{B}}(\mathbf{r},t)$  and  $\dot{\mathbf{D}}(\mathbf{r},t)$  denotes the time derivation,  $\rho \left[\frac{C}{m^3}\right]$  is the volume electric charge density,  $\mathbf{J} \left[\frac{A}{m^2}\right]$  is the vector of electric current density. Because of the high complexity of the problem of light scattering by arbitrary shaped and sized particles that build together powder-like structures with various distributions and densities, this research is restricted to a material classification which is linear, time-invariant and isotropic regarding the applied wavelengths of the incident electromagnetic waves. The relative permittivity is spatial dependent  $\varepsilon_r(\mathbf{r})$  and it possesses a real value for transparent particles and a complex value for the absorbing ones. The relative permeability  $\mu_r = 1$  characterizes non-magnetizable substances. The material properties are then described by the following equations:

$$\mathbf{D}(\mathbf{r}, t) = \varepsilon_0 \varepsilon_r(\mathbf{r}) \mathbf{E}(\mathbf{r}, t)$$
  

$$\mathbf{B}(\mathbf{r}, t) = \mu_0 \mu_r \mathbf{H}(\mathbf{r}, t)$$
  

$$\mathbf{J}(\mathbf{r}, t) = \kappa(\mathbf{r}) \mathbf{E}(\mathbf{r}, t)$$
(2.2)

 $\varepsilon_0 \begin{bmatrix} \frac{As}{Vm} \end{bmatrix}$  and  $\mu_0 \begin{bmatrix} \frac{Vs}{Am} \end{bmatrix}$  denote the permittivity and permeability of vacuum, respectively.  $\kappa(\mathbf{r})$  is the electrical conductivity

Before solving Maxwell equations additional assumptions have been taken into account that there are no electric currents and no free electric charges in the investigated structures, i. e.,  $\mathbf{J}(\mathbf{r}) = \mathbf{0}$ ,  $\rho = 0$ . Considering these assumptions and using 2.2 in 2.1 yield the following simplified form of Maxwell equations:

$$\operatorname{rot} \mathbf{E}(\mathbf{r}, t) = -\mu_0 \mathbf{H}(\mathbf{r}, t)$$
  

$$\operatorname{rot} \mathbf{H}(\mathbf{r}, t) = \varepsilon_0 \varepsilon_r(\mathbf{r}) \dot{\mathbf{E}}(\mathbf{r}, t)$$
(2.3)

The illumination of the studied system is performed by a monochromatic electromagnetic plane wave that propagates in z direction ( see figure 2.1). This means, all electric and magnetic fields oscillate harmonically with the angular frequency  $\omega = kc = 2\pi c/\lambda$ . With the wave number  $k [m^{-1}]$ , the speed of light  $c [\frac{m}{s}]$  and the wavelength  $\lambda [m]$ . Here, it is worthy to define the near and far fields as they will be used in the following formulations for calculating the scattering matrix. The near field is the field close to the surface of the scatterer ( $|\mathbf{r}| \leq \lambda$ ) and the far field is the one, which is at least a few wavelengths far away from the considered body ( $|\mathbf{r}| \gg \lambda$ ).



Figure 2.1: Geometry of light scattering from an object.

#### CHAPTER 2. THEORETICAL BASIS OF LIGHT SCATTERING

After solving Maxwell equations, applying Fourier transformation to the calculated near electric and magnetic fields in the time domain delivers them in the frequency domain ( $\mathbf{E}(\mathbf{r}, \omega)$  and  $\mathbf{H}(\mathbf{r}, \omega)$ ). These near fields then get transformed to the far ones in the next step. The reason of this is having the simulation domain as small as possible for saving computational effort, as the far fields can be calculated from the near ones directly without need to simulate for such big distances. Of course, it is possible to get the far field directly without this transformation. However, the computational domain in this case must be very large, which is redundant and not practical at all. Next, integrating the obtained far fields over the volume of the scattering object or over an arbitrary regular surface surrounding it yields the scattering properties of the scattering system.

In particular, when studying the light scattering for any system in the nature, the measurable quantities in the observations or experiments are the field intensities, i.e., the squares of the distinct electric field components with their additions and differences regarding to the planes that are parallel and perpendicular to the incident one. At this point Stokes vector is defined as  $\mathbf{I}(\mathbf{r},\omega) = (I(\mathbf{r},\omega), Q(\mathbf{r},\omega), U(\mathbf{r},\omega), V(\mathbf{r},\omega))^T$  [24, 25] to describe the polarization state of monochromatic electromagnetic wave. Here  $I(\mathbf{r},\omega)$  is the total intensity,  $Q(\mathbf{r},\omega)$ ,  $U(\mathbf{r},\omega)$  and  $V(\mathbf{r},\omega)$  describe the axis, diagonal and circular degree of polarization, respectively. Each parameter of the Stokes vector is proportional to the sum or subtraction of the intensities of the electric field  $\mathbf{E}$  (see the following equation 2.4). For the incident and scattered light, Stokes vector is given by [24, 25]:

$$I(\mathbf{r},\omega) = \langle E_{\parallel}(\mathbf{r},\omega)E_{\parallel}^{*}(\mathbf{r},\omega) + E_{\perp}(\mathbf{r},\omega)E_{\perp}^{*}(\mathbf{r},\omega) \rangle$$

$$Q(\mathbf{r},\omega) = \langle E_{\parallel}(\mathbf{r},\omega)E_{\parallel}^{*}(\mathbf{r},\omega) - E_{\perp}(\mathbf{r},\omega)E_{\perp}^{*}(\mathbf{r},\omega) \rangle$$

$$U(\mathbf{r},\omega) = \langle E_{\parallel}(\mathbf{r},\omega)E_{\perp}^{*}(\mathbf{r},\omega) + E_{\perp}(\mathbf{r},\omega)E_{\parallel}^{*}(\mathbf{r},\omega) \rangle$$

$$V(\mathbf{r},\omega) = j \langle E_{\parallel}(\mathbf{r},\omega)E_{\perp}^{*}(\mathbf{r},\omega) - E_{\perp}(\mathbf{r},\omega)E_{\parallel}^{*}(\mathbf{r},\omega) \rangle$$

$$(2.4)$$

Where  $E_{\parallel}$  describes the electric field component that is parallel to the incidence plane and  $E_{\perp}$  denotes the perpendicular one. The incident plane here is constructed by the vector of light incidence and the normal vector of the scatterer's surface. The spatially dependent scattered fields  $(E_{\parallel sc}, E_{\perp sc})$  involved in calculating Stokes vector are directly coupled with the incident ones  $(E_{\parallel in}, E_{\perp in})$  by the 2 × 2 amplitude scattering (Jones) matrix  $\mathbf{S}(\mathbf{r}, \omega)$ . The following equation describes this relationship for a monochromatic incident wave that propagates in z direction [24]:

$$\begin{bmatrix} E_{\parallel sc}(\mathbf{r},\omega) \\ E_{\perp sc}(\mathbf{r},\omega) \end{bmatrix} = \frac{e^{jk(r-z)}}{-jkr} \begin{bmatrix} S_a(\mathbf{r},\omega) & S_b(\mathbf{r},\omega) \\ S_c(\mathbf{r},\omega) & S_d(\mathbf{r},\omega) \end{bmatrix} \begin{bmatrix} E_{\parallel in}(\mathbf{r},\omega) \\ E_{\perp in}(\mathbf{r},\omega) \end{bmatrix}.$$
 (2.5)

This equation shows how to obtain the amplitude scattering matrix that describes the optical properties of the system. The incident field is known and the scattered far field needs to be calculated. As mentioned above, this can be attained by internal field integration over the entire particle volume or by integrating the near field over an arbitrary virtual surface around the particle. However, the surface integral delivers accurate results when increasing the refractive index of the structure [72], which is not the case for the volume based one. This surface integration method is applied making use of the electromagnetic equivalent theorem [73] for the purpose of transforming the near field amplitudes to the far field ones. The scattered far electric field  $\mathbf{E}_{sc}(\mathbf{r},\omega)$  belonging to the surface integral in this case is given as:

Here  $\hat{\mathbf{n}}_{sc}$  is the unit vector showing in the direction of the scattered light,  $\partial V$  is the arbitrary chosen integration surface around the particle,  $\hat{\mathbf{n}}$  is the unit vector normal which points outwardly to the surface. The entries of the matrix  $\boldsymbol{\psi}(\mathbf{r},\omega)$ , which represents a form of the amplitude scattering matrix  $\mathbf{S}(\mathbf{r},\omega)$ , can be calculated from the electric and magnetic fields  $\mathbf{E}(\mathbf{r},\omega)$ ,  $\mathbf{H}(\mathbf{r},\omega)$  by surface integration as follows:

where  $\hat{\alpha}$  is the parallel unit vector to the scattering plane, as well  $\hat{\beta}$  is the perpendicular one to the scattering plane (see figure 2 in [51]). Both  $\hat{\alpha}$  and  $\hat{\beta}$  fulfill the condition:

$$\hat{\mathbf{n}}_{sc} = \hat{\boldsymbol{\beta}} \times \hat{\boldsymbol{\alpha}} \tag{2.9}$$

we can obtain the amplitude scattering matrix  $\mathbf{S}(\mathbf{r}, \omega)$  from  $\boldsymbol{\psi}(\mathbf{r}, \omega)$  matrix as derived in [51,72]:

$$\begin{bmatrix} S_a(\mathbf{r},\omega) & S_b(\mathbf{r},\omega) \\ S_c(\mathbf{r},\omega) & S_d(\mathbf{r},\omega) \end{bmatrix} = \begin{bmatrix} \psi_{\hat{\alpha},y}(\mathbf{r},\omega) & \psi_{\hat{\alpha},x}(\mathbf{r},\omega) \\ \psi_{\hat{\beta},y}(\mathbf{r},\omega) & \psi_{\hat{\beta},x}(\mathbf{r},\omega) \end{bmatrix} \begin{bmatrix} \sin(\varphi) & -\cos(\varphi) \\ \cos(\varphi) & \sin(\varphi) \end{bmatrix}.$$
 (2.10)

The spherical coordinates  $\mathbf{r} = (r, \theta, \varphi)$  are taken into account here in order to describe the scattering in all directions. The elements of the amplitude scattering matrix get averaged over the azimuth angle  $\varphi$ , thus, only the spatial dependency of  $\theta$  remains for this matrix  $\mathbf{S}(\theta, \omega)$ .

Consequently, the final field amplitudes represented in  $\mathbf{S}(\theta, \omega)$  are transformed to the intensity quantities for getting the 4 × 4 Mueller matrix (the scattering matrix) [24, 25]. The underlying reason for this transformation is studying the intensity and linear polarization, that are attained from the scattering matrix and are the quantities obtained by photopolarimetric observations and laboratory measurements. The scattering matrix

#### CHAPTER 2. THEORETICAL BASIS OF LIGHT SCATTERING

connects the incidence and scattering Stokes parameters as follows [24, 25]

$$\begin{bmatrix} I_{sc}(\mathbf{r},\omega) \\ Q_{sc}(\mathbf{r},\omega) \\ U_{sc}(\mathbf{r},\omega) \\ V_{sc}(\mathbf{r},\omega) \end{bmatrix} = \frac{1}{k^2 r^2} \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{bmatrix} \begin{bmatrix} I_{in}(\mathbf{r},\omega) \\ Q_{in}(\mathbf{r},\omega) \\ U_{in}(\mathbf{r},\omega) \\ V_{in}(\mathbf{r},\omega) \end{bmatrix},$$
(2.11)

where the entries of the scattering matrix (from  $S_{11}$  to  $S_{44}$ ) depend only on  $\theta$  and  $\omega$ . The intensity is represented by the first element in the scattering matrix  $(S_{11})$  and the polarization degree by  $(-S_{21}/S_{11})$ . Both intensity and polarization are plotted with the scattering angles to evaluate the results of this work (see figures 1.5 and 1.4). As the theoretical background of light scattering has been discussed in this chapter, the next chapter explains how to solve the scattering problem numerically in an efficient way on a high performance computational platform.

## The Discontinuous Galerkin Method in Time Domain (DGTD)

3

The Discontinuous Galerkin method that is employed in this work is a very popular mathematical approach. It is widely used in a plenty of industrial and scientific areas like electrical and mechanical engineering, physics, chemistry, medicine and more (e.g. [65–67,74–91]). In comparison to frequency domain methods, time domain methods allow simulating short pulses with broad spectra in a single simulation. They have the advantage of visualizing the behavior of the physical system and viewing the associated effects of it. Hence, it is easier to understand or interpret its basic dynamics. This supports making further decisions about system design, configuration, and mathematical formulation.

Choosing the DGTD method for performing the computations in this work is due to the efficient parallelizability and scalability of the algorithm on HPC clusters. This is because of the locality of the mathematical operations on the grid elements, i.e., Maxwell's equations are solved in each cell separately. Apart from this, the grid of the simulation domain in this method is unstructured. As a consequence, this allows meshing densely packed irregular shapes in an accurate way efficiently in comparison to the structured meshes. This chapter describes the DGTD method briefly according to the references [64–67].

#### **3.1** Theoretical background and general formulation

The three-dimensional Maxwell's equations in time domain (equations 2.3) can be expressed in a form of the conservation law:

$$\mathbf{Q}(\mathbf{r})\dot{\boldsymbol{\xi}}(\mathbf{r},t) + \nabla \cdot \mathbf{F}(\boldsymbol{\xi}(\mathbf{r},t)) = 0$$
(3.1)

Where  $\mathbf{r} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z$  is the local vector in space and  $\mathbf{Q}(\mathbf{r})$  is the spatially dependent matrix of material constants:

$$\mathbf{Q}(\mathbf{r}) = \begin{bmatrix} \varepsilon(\mathbf{r}) & 0\\ 0 & \mu(\mathbf{r}) \end{bmatrix},$$

where  $\varepsilon(\mathbf{r}) = \varepsilon_0 \varepsilon_r(\mathbf{r})$  is the permittivity,  $\mu(\mathbf{r}) = \mu_0 \mu_r(\mathbf{r})$  is the permeability and  $\boldsymbol{\xi}(\mathbf{r}, t)$  is a single six component vector of unknowns, namely, the electric and magnetic fields  $\mathbf{E}(\mathbf{r}, t)$ ,  $\mathbf{H}(\mathbf{r}, t)$ , respectively:

$$\boldsymbol{\xi}(\mathbf{r},t) = \left[ \begin{array}{c} \mathbf{E}(\mathbf{r},t) \\ \mathbf{H}(\mathbf{r},t) \end{array} \right].$$

 $\mathbf{F}(\boldsymbol{\xi})$  is the flux:

$$\mathbf{F}(\boldsymbol{\xi}) = \begin{bmatrix} \boldsymbol{f}_x(\boldsymbol{\xi}(\mathbf{r},t)) \\ \boldsymbol{f}_y(\boldsymbol{\xi}(\mathbf{r},t)) \\ \boldsymbol{f}_z(\boldsymbol{\xi}(\mathbf{r},t)) \end{bmatrix},$$

where  $f_i(\boldsymbol{\xi}(\mathbf{r},t))$  is defined as:

$$\boldsymbol{f}_{j}(\boldsymbol{\xi}(\mathbf{r},t)) = \left[ \begin{array}{c} -\hat{\mathbf{e}}_{j} \times \mathbf{H}(\mathbf{r},t) \\ +\hat{\mathbf{e}}_{j} \times \mathbf{E}(\mathbf{r},t) \end{array} \right],$$

where  $\hat{\mathbf{e}}_j$  representing the Cartesian unit vectors with  $j \in \{x, y, z\}$ . In the purpose of solving Maxwell's equations for a specific structure numerically, they need to be discretized in space and time.

#### 3.2 Space discretization of the computational domain

Generally, the simulation domain consists of the structure of interest and free space around it, which can be vacuum, air or any material depending on the investigated physical system. This is demonstrated in figure 3.1a, which represents a simple example of a mesh with two close spheres in a cylindrical domain surrounded by vacuum. In addition, the boundaries also belong to the simulation domain and can be just a condition for the fields at its external boundary elements like Dirichlet and Neumann boundary conditions [92– 95], as well the periodical ones [96,97] or they can be defined on an additional surrounding region like in the case of perfectly matched layer (PML) [98–100] as shown in figure 3.1b. Chapter 3. The Discontinuous Galerkin Method in Time Domain (DGTD)



Figure 3.1: Examples of two spatially discretized cylindrical simulation domains of two very close faceted spheres in vacuum (a) and one irregular particle in vacuum surrounded by absorbing perfectly matched layer (b).

Depending on the dimensionality of the studied system, the simulation domain  $\Omega$  is divided into K non-overlapped cells  $\Omega_k$ . These cells can be lines for 1D, faces for 2D or volumes for 3D systems. The mesh can be structured, i.e., its cells or elements have the same shape and size like in the FDTD method [50]. The advantage here is the simple implementation of the mesh generation algorithm associated with simple accessibility to the mesh elements directly through their indices in a simple way. Despite this, when having complex geometries with non-aligned axis topologies or even with curved forms, the structured grids are not flexible enough for representing these geometries and a staircase effect can come out. Highly increasing the spatial resolution can help here, but it is still not the optimal case for treating such structures. Unstructured discretization is an efficient way to deal with such complex shapes. It allows flexible space representation of cubes, faceted spherical and ellipsoidal shapes as well as random irregular particles that is the target geometries in this work. The tetrahedral mesh generator used here is based on the TetGen library [101]. Other examples of the available mesh generation tools are Gmsh [102], NETGEN [103] and libMesh [104]. The TetGen mesh generator discretizes the computational domain into K non-overlapping arbitrary shaped and sized tetrahedral cells  $\Omega_k$  (see figure 3.1). What this figure also shows is the mesh refinement related to different zones separately. This can be achieved by increasing the number of the tetrahedra when decreasing their volumes for special regions (*h-refinement*). Thus, allowing higher accuracy in the region of interest and saving calculation time in regions

where high accuracy is not definitely needed. The two spheres in 3.1a and the irregular particle in 3.1b possess higher resolution than the surrounding medium, which is assumed as vacuum. The reason of this refinement is that the wavelength of the electromagnetic wave propagating in the material of the structure is smaller than it is in vacuum. Thus, smaller cell volumes are required here to stay at the same accuracy for all regions depending on the wavelength and the corresponding refractive index of the material of each cell. In contrast, there is no need for high resolution for the PML region in 3.1b. The reason behind this is that the role of this layer is not to study the electric and magnetic fields there, it is rather to absorb them as possible without getting undesirable reflections. Hence, relatively large cells are able to do this mission successfully, which in turn require less computational effort and save simulation time as well. *h*-refinement is not the only way for controlling accuracy. In DGTD the local solution in each element is expanded in local polynomial basis. Increasing this order p of the polynomial representation ensures higher degree of freedom (larger number of grid points). Thus, a more precise numerical solution is achieved. This is called (*p*-refinement). For each tetrahedral element, an approximated a local polynomial solution  $\tilde{\boldsymbol{\xi}}^{k}(\mathbf{r},t)$  including the electric and magnetic fields, is represented on its nodes as a result of solving Maxwell's equations. The polynomial expression of the numerical solution in each cell is given as a sum over all of its nodes  $\mathcal{N}_{nodes}$  that are positioned at  $\mathbf{r}_i$  as:

$$\tilde{\boldsymbol{\xi}}^{k}(\mathbf{r},t) = \sum_{n=1}^{\mathcal{N}_{nodes}} \tilde{\boldsymbol{\xi}}_{n}^{k}(t) \eta_{n}(\mathbf{r}) = \sum_{i=1}^{\mathcal{N}_{nodes}} \tilde{\boldsymbol{\xi}}^{k}(\mathbf{r}_{i},t) \mathcal{L}_{i}(\mathbf{r}).$$
(3.2)

Here,  $\tilde{\boldsymbol{\xi}}_n^k$  are the expansion coefficients,  $\eta_n(\mathbf{r})$  is a local polynomial basis,  $\mathcal{L}_i(\mathbf{r})$  are Lagrange polynomials.

The total number of nodes  $(\mathcal{N}_{nodes})$  for each cell is related to the dimension 1D, 2D or 3D and the order p of Lagrange polynomials  $\mathcal{L}_i$  that are utilized to represent the numerical solution. At each node Lagrange polynomial has a non-zero value for it, whereas for all other nodes of the tetrahedron, it has a zero one. The following expressions represent the number of nodes that are needed for each dimension depending on the polynomial order:

1D	$\mathcal{N}_{nodes} = p + 1$
2D	$\mathcal{N}_{nodes} = (p+1)(p+2)/2$
3D	$\mathcal{N}_{nodes} = (p+1)(p+2)(p+3)/6$

As example, for a three dimensional computational domain, if the order the expansion terms is one (p = 1), the unknown fields will be only computed on the four vertices of each tetrahedron. In this work, the used polynomial order is p = 3. This can provide accuracy if sufficient mesh resolution is chosen. Hence,  $\mathcal{N}_{nodes} = 20$  nodes are involved in each tetrahedron to represent the solution as figure 3.2 illustrates.

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Figure 3.2: Representation of the electric **E** and magnetic **H** field components on all element nodes for the polynomial order p = 3 of the expansion.

#### 3.3 Derivation of the semi-discrete numerical scheme

Maxwell's equations in conservation form (equation 3.1) are approximately satisfied by the local numerical solution  $\tilde{\boldsymbol{\xi}}^{k}(\mathbf{r},t)$  for each cell. This means that the right hand side will have a residual  $\tilde{\mathcal{R}}(\mathbf{r},t)$  when solving the problem numerically, instead of zero for an analytical solution. This residual will take place in equation 3.1 as given by the expression:

$$\mathbf{Q}(\mathbf{r})\tilde{\boldsymbol{\xi}}^{k}(\mathbf{r},t) + \nabla \cdot \mathbf{F}(\boldsymbol{\xi}) = \tilde{\mathcal{R}}(\mathbf{r},t).$$
(3.3)

For a good convergence to accurate solution the residual must be minimized by multiplying with orthogonal test functions that are also Lagrange polynomials  $\mathcal{L}_i$  for each cell node *i* to satisfy:

$$\int_{\Omega^k} \left( \mathbf{Q}(\mathbf{r}) \dot{\boldsymbol{\xi}}^k(\mathbf{r}, t) + \nabla \cdot \mathbf{F}(\tilde{\boldsymbol{\xi}}^k) \right) \mathcal{L}_i(\mathbf{r}) d^3 r = \int_{\Omega^k} \tilde{\mathcal{R}}(\mathbf{r}, t) \mathcal{L}_i(\mathbf{r}) d^3 r \longrightarrow 0.$$
(3.4)

Choosing the test functions the same as the interpolation polynomials is called Galerkin approach. The residual must be orthogonal to the function space spanned by  $\mathcal{L}_i(\mathbf{r})$ . Now this is an equation for local numerical solutions for each element. The global numerical solution is achieved by collecting the local discontinuous ones together as follows:

$$\tilde{\boldsymbol{\xi}}(\mathbf{r},t) = \bigoplus_{k=1}^{K} \tilde{\boldsymbol{\xi}}^{k}(\mathbf{r},t).$$
(3.5)

The issue that the local solutions are calculated separately does not guarantee that these solutions are continuous, i.e., they can be not matching or have some shifting to each other on the element's boundary. At this point the numerical flux  $\mathbf{F}^*(\tilde{\boldsymbol{\xi}}^k)$  is defined. The purpose of this flux is taking the discontinuity into account and involving the fields belonging to the neighbor elements on the shared boundary in the local operations. In order to include  $\mathbf{F}^*(\tilde{\boldsymbol{\xi}}^k)$  into the equation 3.4 two steps must be done. Performing partial integration of 3.4 delivers a volume integral on the left hand side and an integral over all surfaces of the tetrahedral element on the other side:

$$\int_{\Omega^k} \left( \mathbf{Q}(\mathbf{r}) \dot{\tilde{\boldsymbol{\xi}}}^k(\mathbf{r}, t) \mathcal{L}_i(\mathbf{r}) - \mathbf{F}(\tilde{\boldsymbol{\xi}}^k) \cdot \nabla \mathcal{L}_i(\mathbf{r}) \right) d^3 r = - \oint_{\partial \Omega^k} \left( \mathbf{\hat{n}} \cdot \mathbf{F}(\tilde{\boldsymbol{\xi}}^k) \right) \mathcal{L}_i(\mathbf{r}) d^2 r, \qquad (3.6)$$

where  $\hat{\mathbf{n}}$  is the normal of the local element face and points outwardly. Subsequently, applying partial integration again gives the left hand side back in its original expression, but on the right hand side, a subtraction between the flux  $\mathbf{F}(\tilde{\boldsymbol{\xi}}^k)$  and the numerical flux  $\mathbf{F}^*(\tilde{\boldsymbol{\xi}}^k)$  is obtained as the following equation shows:

$$\int_{\Omega^k} \left( \mathbf{Q}(\mathbf{r}) \dot{\tilde{\boldsymbol{\xi}}}^k(\mathbf{r}, t) + \nabla \cdot \mathbf{F}(\tilde{\boldsymbol{\xi}}^k) \right) \mathcal{L}_i(\mathbf{r}) d^3 r = \oint_{\partial \Omega^k} \mathbf{\hat{n}} \cdot \left( \mathbf{F}(\tilde{\boldsymbol{\xi}}^k) - \mathbf{F}^*(\tilde{\boldsymbol{\xi}}^k) \right) \mathcal{L}_i(\mathbf{r}) d^2 r \qquad (3.7)$$

The additional surface integral here on the right hand side involves the field differences  $\Delta \mathbf{E}$  and  $\Delta \mathbf{H}$  between the element itself and its neighboring element. This has the task of matching the local solutions between the elements after choosing appropriate numerical flux as described in [65]. In other words, the numerical flux is used for adjusting of the discontinuous solutions to match each other on the boundary of each tetrahedron with the surrounding tetrahedra. This is an important step to get an approximate global continuous solution from discontinuous local ones. Obviously, it causes extra computational effort for more operations and memory consumption. However, this is the cost of having discontinuous solutions, which is the advantage for parallelization of the numerical algorithm. According to the derivation described in [65, 66], the semi-discrete Maxwell's equations are obtained in the following formulations:

$$\epsilon^{k} \dot{\mathbf{E}}^{k} = \mathcal{D}^{k} \times \mathbf{H}^{k} + (\mathcal{M}^{k})^{-1} \mathcal{F}^{k} \frac{1}{\overline{Z}} \left( \Delta \mathbf{E} - \hat{\mathbf{n}} \cdot (\hat{\mathbf{n}} \cdot \Delta \mathbf{E}) + Z^{+} \hat{\mathbf{n}} \times \Delta \mathbf{H} \right)$$
(3.8)

$$\mu^{k}\dot{\mathbf{H}}^{k} = -\boldsymbol{\mathcal{D}}^{k} \times \mathbf{E}^{k} + (\mathcal{M}^{k})^{-1}\mathcal{F}^{k}\frac{1}{\overline{Y}}\left(\Delta\mathbf{H} - \mathbf{\hat{n}}\cdot(\mathbf{\hat{n}}\cdot\Delta\mathbf{H}) - Y^{+}\mathbf{\hat{n}}\times\Delta\mathbf{E}\right)$$
(3.9)
#### CHAPTER 3. THE DISCONTINUOUS GALERKIN METHOD IN TIME DOMAIN (DGTD)

Here the left hand side represents the time derivative of the electric and magnetic fields multiplied with the material constants,  $\mathcal{D}^k = (\mathcal{D}^k_x, \mathcal{D}^k_y, \mathcal{D}^k_z)$  is the spatial differentiation matrix, where  $\mathcal{D}^k_{l_{ji}} = \partial_l \mathcal{L}_i(\mathbf{r}_j)$ ,  $l \in \{x, y, z\}$ ,  $\mathcal{M}_{ji} = \int_{\Omega^k} \mathcal{L}_j(\mathbf{r}) \mathcal{L}_i(\mathbf{r}) d\mathbf{r}$  is the mass matrix,  $\mathcal{F}_{ji} = \oint_{\partial\Omega^k} \mathcal{L}_j(\mathbf{r}) \mathcal{L}_i(\mathbf{r}) d\mathbf{r}$  is the face matrix, and as mentioned above,  $\Delta \mathbf{E}$  and  $\Delta \mathbf{H}$ (see figure 3.4) are the field differences at the shared points between each two neighboring cells [66]. They are calculated as follows:

$$\Delta \mathbf{E}(\mathbf{r},t) = \mathbf{E}^{+}(\mathbf{r},t) - \mathbf{E}^{-}(\mathbf{r},t)$$
(3.10)

$$\Delta \mathbf{H}(\mathbf{r},t) = \mathbf{H}^{+}(\mathbf{r},t) - \mathbf{H}^{-}(\mathbf{r},t)$$
(3.11)

The impedance is represented by

$$Z^{\pm} = \sqrt{\mu \pm /\varepsilon \pm}$$

and the conductance

$$Y^{\pm} = (Z^{\pm})^{-1} = \sqrt{\varepsilon \pm /\mu \pm} .$$

Both define material parameters for each mesh element. The current cell, for which computations are performing, is denoted with "-", and "+" denotes the neighbor one. The sums of them are:

$$\overline{Z} = Z^+ + Z^-$$

and

$$\overline{Y} = Y^+ + Y^-.$$

In order to simplify the computations, the differentiation matrix  $\mathcal{D}^k$ , the mass matrix  $\mathcal{M}$ and the face matrix  $\mathcal{F}$  are computed only once for a reference element in the Cartesian coordinates system  $(\hat{x}, \hat{y}, \hat{z})$ . They get linearly transformed from the Cartesian coordinates system (x, y, z) for each tetrahedron in the mesh using Jacobian transformation. Consequently, this saves memory consumption and computation time [67]. This affine transformation for mesh elements is represented in figure 3.3 for 1D, 2D and 3D grids.



Figure 3.3: Affine transformation of the mesh cells into a reference element for one, two and three dimensional grid using two Cartesian coordinates systems (x, y, z) and  $(\hat{x}, \hat{y}, \hat{z})$ .

#### 3.4 Explicit time stepping

As discrete scheme for Maxwell's equations has been derived, the only step left to get the equation system as a numerical scheme is time integration. There are many time stepping techniques that can be categorized in implicit and explicit methods. The explicit low storage Runge-Kutta method (LSRK) [65–67, 105–107] is employed in the numerical scheme of the DGTD solver used here. It turns out to be an adequate choice because it is memory efficient. A relatively small time step must be chosen due to the Courant condition in order to get acceptable accuracy and numerical stability. Larger time step can lead to growing of the evaluated unknowns exponentially after each iteration in the solver, which must be definitely avoided. As a criteria for numerical stability, the time step  $\Delta t$  in DGTD is chosen regarding to the shortest distance between two grid points in the mesh [66,67]. It is expressed as follows:

$$\Delta t_{\max} \leqslant s \cdot d_{\min}(p) \cdot \min(r_{\min}^{\Delta}), \qquad (3.12)$$

where s is a factor that has the order of 1 and can be chosen according to the problem of interest and the used numerical scheme,  $d_{\min}(p)$  is the shortest distance in the mesh between two neighbor nodes,  $r_{\text{in}}^{\Delta}$  is the radius of the inscribed sphere in the mesh cell.

After each iteration, the unknown fields are executed by solving Maxwell's equations. The LSRK requires only two storage locations for each unknown, namely,  $\tilde{\xi}$  and  $\tilde{\xi}_{res}$ . As the ordinary differential equations of the semi-discrete scheme take the form:

$$\tilde{\boldsymbol{\xi}}^k(\mathbf{r},t) = \mathbf{g}(\tilde{\boldsymbol{\xi}}^k(\mathbf{r},t),t).$$

The LSRK-scheme for one unknown or one field component of the numerical solution for a time step starting from the step m to m + 1 is given as:

$$\begin{split} \tilde{\xi}(\mathbf{r},t) &= \tilde{\xi}(\mathbf{r},t_m), \\ \tilde{\xi}_{res_n}(\mathbf{r},t,\Delta t) &= A_n \tilde{\xi}_{res_{n-1}} + \mathbf{g}(\tilde{\xi}_{n-1},t_m+C_n\,\Delta t)\Delta t \\ \tilde{\xi}_n(\mathbf{r},t) &= \tilde{\xi}_{n-1}(\mathbf{r},t) + B_n \tilde{\xi}_{res_n}(\mathbf{r},t,\Delta t), \\ \tilde{\xi}(\mathbf{r},t_{m+1}) &= \tilde{\xi}(\mathbf{r},t), \end{split} \right\} n = 1,2,\dots,N_{RK-stages}$$

where  $N_{RK-stages}$  is the number of Runge-Kutta stages,  $A_n, B_n$  and  $C_n$  are the Runge-Kutta constants [67, 105]. The implemented time stepping in the DGTD solver for this work is the optimized 4th order LSRK method with 14 stages as described in [105]. This delivers faster results in comparison with the traditional 4th order one with 5 stages (see [66, 105]).

The last step for solving a real-world problem is implementing a light source function. Here, field values are incorporated at a specific point or set of points of interest in the simulation domain as a space and time dependent function. This means that the illumination will be injected continuously as long as the simulation is performed. In order to simulate light scattering from an object of interest, a monochromatic electromagnetic plane wave is injected in the simulation domain. Only the scattered fields are interesting to get the scattering properties of the investigated system as mentioned in chapter 2. Therefore, the computational domain is divided into two regions, namely, the total and the scattered regions that are illustrated in figure 3.4. The incident field must be subtracted from the total one at each tetrahedron belonging to the scattered field region. This is called the total field/scattered field technique (TF/SF) [50,67]. The electric and magnetic fields are given as:

$$\begin{aligned} \mathbf{E}_{tot}(\mathbf{r}, t) &= \mathbf{E}_{in}(\mathbf{r}, t) + \mathbf{E}_{sc}(\mathbf{r}, t) \\ \mathbf{H}_{tot}(\mathbf{r}, t) &= \mathbf{H}_{in}(\mathbf{r}, t) + \mathbf{H}_{sc}(\mathbf{r}, t), \end{aligned}$$

where  $\mathbf{E}_{tot}(\mathbf{r}, t)$ ,  $\mathbf{H}_{tot}(\mathbf{r}, t)$  are the total electric and magnetic fields, respectively. The electric field differences at TF/SF boundary are calculated using equation 3.10 as follows:

$$\Delta \mathbf{E}_{tot}(\mathbf{r}, t) = \mathbf{E}_{sc}^{+}(\mathbf{r}, t) - \mathbf{E}_{tot}^{-}(\mathbf{r}, t) + \mathbf{E}_{in}(\mathbf{r}, t)$$
$$\Delta \mathbf{E}_{sc}(\mathbf{r}, t) = \mathbf{E}_{tot}^{+}(\mathbf{r}, t) - \mathbf{E}_{sc}^{-}(\mathbf{r}, t) - \mathbf{E}_{in}(\mathbf{r}, t).$$



The same calculation approach is valid for the magnetic field.

Figure 3.4: Representation of a simulation domain with total field / scattered field regions and field differences between the interface nodes of two neighboring tetrahedrons.

### 3.5 Parallelized DGTD code

The DGTD solver employed in this work take advantage of the MPI library [108] and can be executed on multiple CPU cores. The ParMetis library [109] is used in order to partition the mesh, where each mesh part gets assigned to a MPI process that perform the computations for the appropriate partition. When data exchange between partitions is required for arithmetic operations, the processes communicate with each other using MPI message passing interface. This occurs at the boundary of spatial neighboring grid parts, allowing for calculating the flux. This requires preparation of mapping matrices as it will be described in the next section.

#### 3.5.1 Mapping between the neighboring elements

In general, communication or data exchange between neighboring cell nodes at the interfaces is required. For programming the flux terms in DGTD method the nodes must

#### Chapter 3. The Discontinuous Galerkin Method in Time Domain (DGTD)

be mapped to each other regarding to their positions and connectivity. Having spatial flexibility to represent complex geometry is a great benefit of unstructured grids. Yet, in order to explain the principle of the mapping between various mesh elements, it makes sense to show this for only one tetrahedron and after that the further steps will be the same for all mesh cells. On one side, the indices of the mesh cells are global and are saved sequentially in a matrix. On the other side, there is another matrix to save the global indices of the neighboring cells appropriately. This is all what is needed for computing the field differences at the cells interfaces and for gathering the discontinuous local solutions into a global continuous one. In contrast to structured grids, unstructured ones need more implementation effort for managing all data exchange between the neighbor elements correctly.

As an example, to clarify the mapping strategy in DGTD, a tetrahedron with order p = 3 is considered. Each tetrahedron of this order has 20 nodes that get global sequential indices. The first cell has indices from 0 to 19 as the numbers inside the circles demonstrate in figure 3.5.



Figure 3.5: The first element of a tetrahedral mesh with its all global indices represented in the circles and only 10 local ones, which belong to its first face on the right hand side and take the numbers from 0 to 9 in the blue rectangles.

The second one has indices from 20 to 39 and so forth for all mesh elements. Then, the first 10 nodes of the first face get new sequential local indices starting from 0 to 9, as can be also seen in the blue rectangles in figure 3.5. Similarly, the nodes of the second face of the same element, which is the back side in this example, get the next sequential set of indices from 10 to 19 as figure 3.6 displays.



Figure 3.6: The first element of a tetrahedral mesh with its all global indices represented in the circles and the first 20 local ones, which belong to its first and second faces on the right hand side and on the back, respectively. The local indices take the numbers from 0 to 19 in the blue and green rectangles appropriately.

Analogously, the nodes of the third and fourth face get the next two sequences of indices. Figure 3.7 displays a full surface indexing of the first mesh cell in the computational domain. It is also noticeable in this figure that each node can take from one up to three distinct indices with respect to the different faces. For instance, the node 0 is shared with three faces of the same element and gets, therefore, three face indices (0, 10 and 30), while the node 11 has just one face node index (15) because it lies in the center of the second face. However, in three-dimensional simulations, for polynomial order higher than three not all nodes will lie on the cell surface. Hence, there will be nodes inside the volume that do not get this new indexing at all. Again, when considering the second mesh

#### Chapter 3. The Discontinuous Galerkin Method in Time Domain (DGTD)

element, it is subject to the same indexing. As a result, although two neighbor cells share the same face spatially, they do not share the nodes computationally, i.e., on the shared surface between two mesh elements, each of them has a full set of face nodes that are neighbored with the ones of the other face. In fact, this consumes more than the double number of memory registers for surface nodes in comparison to the same mesh treated with FEM method. Surface nodes on edges can be shared by more than two tetrahedrons. Nevertheless, this is the cost of the discontinuity in DGTD, which is an essential feature for suitability of the method for parallelization.



Figure 3.7: The first element of a tetrahedral mesh with its all 20 global indices represented in the circles and all local ones, which take the numbers from 0 to 39 in the colored rectangles regarding to the faces appropriately.

All these mapping data, the global and local indices distributed on the element surface of figure 3.7, can be included in a matrix. Figure 3.8 displays how to organize this for the first and second cell of a tetrahedral grid in a simple way. Obviously, the faces indices (the colored ones) are local and belong only to one mesh element. In contrast, the global ones are shared with the neighboring elements. At this point it is possible to put all mapping data of all mesh cells in two connecting matrices, one for the current elements and the another for the neighbors. That is, computational operations can exchange the data using these connection matrices for calculating the field differences and then the flux on the cells boundaries.

1 <sup>st</sup> element of the mesh:	0	1	2	3	4	5	6	7	8	9	
	0	1	2	3	4	5	6	7	8	9	
faces [4] [10] -	10 0	11 1	12 2	13 3	14 10	15 11	16 12	17 16	18 17	19 19	
laces [4] [10] –	20	21	22	23 9	24 12	25 14	26 15	27 17	28 18	29 19	
	30	31	32	33	34	35	36	37	38	39	
l	0	4	7	9	10	13	15	16	18	19	



Figure 3.8: Connection index matrices of the surface nodes that belong to the first two tetrahedrons of a mesh. The rectangles filled with colors include the 40 sequential matrix indices that represent the indices of tetrahedron faces. Each line represents one face with the appropriate color used in figure 3.7. The 20 global indices are represented as values of the mapping matrix. They don't necessarily have to be in sequential order here like the other ones of faces.

The discontinuity is a significant property of DGTD as the mathematical operations are performed on each single mesh element separately instead of dealing with global matrices like the case of the FEM method. The issue that each grid element has its own nodes and relatively small number of local calculations suggests DGTD as a suitable simulation method for parallelization in order to run on heterogeneous high performance computing platforms.

# 4

## Numerical model

#### 4.1 Model description

In this section the model geometries that are used as target objects are discussed. These are single particles and pairs of particles of different shapes for studying double scattering. As well monolayers of spheres and irregular particles are investigated to study multiple scattering. A full wave electromagnetic problem is solved employing DGTD method that is described in chapter 3. The considered constituent shapes are cubes, faceted spheres and ellipsoids with diverse aspect ratios, as well as, random irregular particles. For the last case, Gaussian random field (GRF) shapes [27,110] have been utilized. Figure 4.1 demonstrates six samples of irregular particles. Additionally, for some cases, the separation between the particles have been also explored from nearly touching particles to distances comparable to the scale of one particle size. The particles have sizes much larger than the wavelength of the incident light. A dimensionless size parameter value is used to describe the geometrical sizes of the particles. It is expressed as follows:

$$kR = \frac{2\pi R}{\lambda},\tag{4.1}$$

where k is the wave number and R is the radius of the circumscribing sphere around the particle.

#### 4.1 Model description



Figure 4.1: Samples of randomly oriented irregular GRF particles (a) to (f)

The constituents have size parameter between 20 and 30 regarding to the considered case. The material, the particles consist of, is absorbing for the most cases studied in this work. Transparent particles have been briefly investigated for comparing with absorbing ones. Absorption is controlled by variation of the imaginary part of refractive index m between 0.3 for highly absorbing and 0 for transparent constituents. Increasing the imaginary part of m reduces the contribution of multiple scattering. Furthermore, the real part of refractive index is also considered for both values 1.3 and 1.8 in addition to 1.5.

Designing a powder model is a quite complex problem. Agglomerates of densely packed irregular particles are modeled by applying Bullet physics engine [111]. This is an open source library to simulate three dimensional dynamics and collisions between various rigid bodies. An advantageous point here is the ability to set the mass and friction of each particle. Thus, creating arbitrary types of clusters with the desired high densities. The GRF particles build a cluster together when simulating their free fall into a cylinder without overlapping with each other. In scope of this work an own code for building clusters of particles controlling their number, sizes, distribution and the distances between them have been implemented. This implementation enables random selection of a big set of individual irregular particles for assembling hundreds of cluster samples, where each sample is an agglomerate of a few irregular particles with random orientations. The necessity for a lot of cluster samples, that can reach more than 300 for an individual case study, is justified by averaging all simulation results. As the measured quantities Chapter 4. Numerical model

in laboratory experiments and photopolarimetric observations are obtained from many groups of particles, one needs to average them over a lot of samples in the theoretical study of a scattering system. Thus, numerical computations support the understanding and interpretation of these measurements. The model uses an unpolarized plane wave light source. Figure 4.2 represents the model by a monolayer of 10 irregular densely packed GRF particles.



Figure 4.2: The model represented in a monolayer of 10 densely packed irregular GRF particles

This model is valid also for all regular and irregular shapes used in this work. The unpolarized light source is modeled by two simulation runs with linearly polarized electromagnetic waves with orthogonal polarization to each other. Additionally, as a boundary condition, a perfectly matched layer is used to mimic light scattering in an open infinite space. Figure 4.3 demonstrates a xy cross section in the simulation domain. The particles are positioned very closed to each other in such a way that every one lies in the near field zone of the neighbored one. The agglomerates of particles are surrounded with vacuum. Total field / scattered field (TF/SF) technique as explained in chapter 3 has been employed. The TF/SF zone around the vacuum is the region, in which the electromagnetic fields are measured and integrated in the purpose of calculating the far field, and consequently, the scattering matrix of the system.



Figure 4.3: A cross section in xy plane of the simulation domain for a monolayer of 10 irregular densely packed GRF particles

Figure 4.4 displays a cross-section of a monolayer of ten GRF particles and the distribution of the electric near field components  $E_x$  and  $E_y$  in this layer at the steady-state.



Figure 4.4: Cross-section of the electric near field components  $(E_x \text{ and } E_y)$  and a monolayer of ten irregular particles. The incident field is  $E_y$  polarized.

#### 4.2 Convergence test

Numerical simulations of any physical system must be validated through a convergence test. It is beneficial to implement a simulation software that models the behavior of the system for solving a scientific problem. However, the decisive criterion for this software is delivering correctly approximated results. When preparing a numerical simulation, there are physical and numerical parameters that have to be set in order to get trustworthy results. The grid resolution is one highly important parameter to be appropriately modified. On the one hand, increasing of grid resolution too much is undesirable because this increases the number of the grid elements causing heavier calculation and longer simulation time. On the other hand, decreasing the spatial resolution saves some simulation time but could influence the resulting accuracy, when the grid is too rough. Therefore, a compromise must be taken in order to obtain as accurate results as possible in reasonable simulation time with the available computational capability. The same applies to time discretization.



Figure 4.5: Scattering angle curves of normalized intensity in logarithmic scale (a) and linear polarization (b) for an irregular particle structure with different spatial resolutions. The particle is absorbing with refractive index m = 1.5 + i0.3 and size parameter kR = 30.

In figure 4.5 the spatial resolution of the mesh is analyzed for an irregular absorbing particle with size parameter kR = 30 and refractive index m = 1.5 + i0.3. The number of tetrahedra per wavelength is varied from 2.5 to 5 cells in a step of 0.5. For the normalized intensity curve 3 cells seem to be precise enough for further simulations. However, since polarization at backscattering is more sensible for mesh resolution as can be seen in figure 4.5b, 3 and 3.5 cells per wavelength can be not accurate enough. Hence, four cells

provide good approximation, when compared with higher resolutions. Therefore, 4 cells per wavelength is accepted for all numerical simulations in this work.

Another aspect that must be studied for the convergence is the light pulse duration. Since the structure is continuously illuminated by an unpolarized light, the number of the pumped waves determine the simulation time. The pulse duration depends directly on the size of the considered system, and correspondingly, the size of the simulation domain. The steady state of the simulated system must be achieved, so that increasing the pulse duration does not affect the simulation result any more. For this goal a structure of two irregular particles has been studied, each has a size parameter kR about 30. The incident electromagnetic wave must travel over the entire simulation domain. That is, the pulse duration, or in other words, the number of the wave oscillations must be sufficient to pass the investigated constituents and scatter in all directions. Thus, starting from less than 20 oscillations does not deliver reasonable results for the system size parameter, which is around 60 for a cluster of two close particles. Figure 4.6 displays a scan for the illumination oscillations starting from 20 to 45 ones with a step of 5 and shows that 20 are sufficient here.



Figure 4.6: Scattering angle curves of normalized intensity in logarithmic scale (a) and linear polarization (b) for a sample consisting of two irregular particles that are close to each other. Each one has a size parameter of kR = 30 and refractive index m = 1.5 + i0.3. One oscillation means one period of the incident wave.

In order to check this, testing another cluster of two irregular particles with same conditions is done. Figure 4.7 demonstrates that 25 oscillations of the incident light are acceptable and deliver converged results that do not get affected when having longer pulse. Hence, 25 oscillations are used to perform computations for scattering systems of such

#### Chapter 4. Numerical model

size, as intensity and polarization curves converge. Consequently, choosing higher number of oscillations for illuminating the cluster here does not give any benefit and associates with unfavorable increased simulation time. Anyway, in case of studying larger clusters or less absorbing particles, the number of oscillations of the incident light must be taken into account, and maybe, increased appropriately.



Figure 4.7: Scattering angle curves of normalized intensity in logarithmic scale (a) and linear polarization (b) for another sample of two irregular particles with kR = 30 and m = 1.5 + i0.3. One oscillation means one period of the incident wave.

Yet, for the purpose of simulating the open boundary conditions, PML must be able to absorb the electromagnetic wave without reflecting it back into the computational domain. This absorption power of the PML boundary is also examined. The thicker PML is, the higher is the absorption of the electromagnetic waves in the boundary. At the same time, the heavier the calculation become, which results in longer simulation time. Figure 4.8 shows that the normalized intensity and linear polarization curves for a PML thickness equivalent to 3 wavelengths converge in comparison with the ones that possess higher thickness values (6 and 11 wavelengths). Thus, a thickness of 3 wavelengths is chosen for the PML boundary.

After setting the numerical and physical parameters of the simulation. A comparison with an analytical solution is targeted. For this purpose the Mie theory is used. Both figures 4.9 and 4.10 display a high matching between results of DGTD code and Mie calculator for single spheres with size parameters kR = 28.3 and 56.6, respectively. The spheres consist of absorbing material with refractive index m = 1.5 + i0.3.



Figure 4.8: Scattering angle curves of normalized intensity in logarithmic scale (a) and linear polarization (b) for a sample consisting of two irregular particles that are close to each other with different PML thicknesses  $(3\lambda, 6\lambda \text{ and } 11\lambda)$ . Each one has a size parameter of kR = 30 and refractive index m = 1.5 + i0.3.



Figure 4.9: Scattering angle curves of normalized intensity in logarithmic scale (a) and linear polarization (b) for single sphere with size parameter kR = 28 calculated with DGTD and a Mie solver.

#### Chapter 4. Numerical model



Figure 4.10: Scattering angle curves of normalized intensity in logarithmic scale (a) and linear polarization (b) for single sphere with size parameter kR = 57 calculated with DGTD and a Mie solver.

#### 4.2 Convergence test

# 5

# Simulation results

The simulations in this work begin with simplified structures of a few particles to check if the negative polarization appears in such systems. The double scattering is apparently responsible for negative polarization in these simple clusters. This is confirmed from double scattering approximate models, which study point scatterers with various single scattering properties like Fresnel scatterers [36,37], electric dipoles that are randomly distributed [38] or particles with Rayleigh polarization phase function [39]. Further developed models of double scattering are also investigated for scattering from a cloud of randomly oriented facets that reflect according to Fresnel formulas [43] or systems of two spherically curved surface elements [112]. Additionally, simple structures allow separating the effects of single and double scattering so that the analysis becomes easier. Therefore, the scattering systems studied were further simplified by using just two particles to constitute the geometry. To consider double scattering, the negative polarization must be studied in detail for different special cases. The considered structures are simplified systems of irregular particles, cubes, ellipsoids with different aspect ratios and different numbers of spheres. The following sections show the types of particles that were used in the simulations.

#### 5.1 Structures of one, two and three GRF particles

Modeling of powder-like systems is a highly complex problem when trying to consider realistic models because of the time consuming design and computational effort. In nature, the neighboring powder particles are touching each other. Modeling touching constituents in numerical simulations is difficult to achieve. This is because the simulation time step depends on the smallest distance between two nodes of the simulation domain. Hence, too small time step comes out, which strongly affects the simulating time making such computations unfeasible or even not possible. Therefore, this must be taken into account for determining the separation between particles. It was possible to find a compromise that the particles are very close to each other with minimum distance much smaller than the wavelength of incident light, and at the same time, reasonable time step still has been achieved. Considering the computational effort, starting from a few GRF particles makes sense in order to check if small cluster of particles is able to produce the negative polarization and the intensity surge at backscattering. Therefore, systems of two, three and ten randomly oriented, irregularly shaped, unique particles are investigated as a simplified powder model [113]. The size parameter of each one is kR = 30. The material is absorbing with refractive index of m = 1.5 + i0.3. Figure 5.1 displays samples of these constituent particles.



(c) Sample one of three irregular particles



Figure 5.1: Samples of two and three irregular GRF particles separated with minimum distances much smaller than the wavelength  $\lambda$  of the incident light.

Figure 5.2 shows the normalized intensity and the linear polarization of structures of two and three irregular particles compared with single-scattering curves, where there is no appearance of the negative polarization, which is expected to get for this instance. Two GRF particles separated with minimum distance much smaller than the wavelength  $\lambda$  show a very small negative polarization at backscattering. Having a separation of approximately the size of one particle between them keep obtaining the weak negative polarization as well. Thus, increasing the distance here does not remarkably affect the

#### Chapter 5. Simulation results

negative polarization. Moreover, a densely packed cluster of three GRF particles is able to enhance the negative polarization near backscattering (see figure 5.2d).



Figure 5.2: Scattering angle curves of (a), (c) normalized intensity in logarithmic and linear scale, respectively, and (b), (d) linear polarization degree. The curves are calculated for single, two and three irregular particles with minimum distance between them, much smaller than the wavelength of incident light, and two particles with separation around one particle size. The constituents consist of absorbing material with refractive index m = 1.5 + i0.3 and size parameter of kR = 30.

This can be clarified by increasing the double-scattering relative contribution to the total scattered field. In other words, the number of possible double-scattering trajectories is tripled, when adding the third particle and quadrupled with additional one. Light

scattering by systems composed of uniquely shaped particles is a stochastic process and the result should be averaged over tens or hundreds of simulations. One or two hundred computations, and in some cases more, have been done in order to get the averaged intensity and linear polarization curves. Single curves for some random samples include only information about that individual sample and do not deliver general characterization directly. Despite of that, analyzing some single curves is relevant and raises some interesting questions or maybe offer some considerable explanation [114]. The motivation for this special consideration are the curves displayed in figure 5.3.



Figure 5.3: Scattering angle curves of (a), (c) normalized intensity in logarithmic and linear scale, respectively, and (b), (d) linear polarization degree gained from four distinct samples of two close irregular particles.

#### Chapter 5. Simulation results

These four curves belong to four different samples of two GRF particles with minimum distance between them. They show a possibility of having no polarization, a strong negative polarization, as well as, positive polarization at backscattering (figures 5.3b and 5.3d). Interestingly, the intensity surge in figures 5.3a and 5.3c does not tend to correlate with the negative polarization or the positive one. Nevertheless, it seems to be more corresponded to the case of having nearly no polarization in figure 5.3d. The reason behind this could be reduced constructive interference of the scattered near fields of second-order for a particular random orientation of the scattering faces and their slopes. This means that the particles produce strong and dominating single scattering for this particular case. At this point irregular particles are not the optimal shapes for investigating the geometry effect. Therefore, structures of two cubes that lie near each other with controlled orientations of their reflecting surfaces are considered. This offers a simplified model for going deep into details to explain the role of geometry on opposition phenomena.

#### 5.2 Structures of two cubes

Here, the double scattering in a symmetric system consisting of two cubic particles is studied. This system constructs corners  $\gamma$  between the reflecting faces of both scatterers ranging from 0° to 180° as figure 5.4 demonstrates.



Figure 5.4: Symmetric two-cube structure builds an angle  $\gamma$  between reflecting surfaces.

Both cubes are separated with a fixed distance much smaller than the wavelength of the incident light. Simulations for this system with changing the angle  $\gamma$  in 1° steps ranging from  $\gamma = 0^{\circ}$  to 180°. Analyzing the results of the single curves shows some common features for different angular ranges of  $\gamma$  regarding to the negative polarization and intensity surge. One can classify the results into six categories or sequences depending on  $\gamma$ , each represents the ascending range of angles between 0° and 180°. This categorization is displayed in figures 5.5 and 5.6 for the normalized intensity and linear polarization, respectively.

The intensity curves illustrate a strong single reflection from the cube surfaces at backscattering, they achieve the highest maximum in two ranges (sequence  $0^{\circ} - 30^{\circ}$  and  $150^{\circ} - 180^{\circ}$ ), since two cubes construct maximum areas of the back-reflecting surfaces in both cases. The direction of single reflection moves to larger scattering angles and after that backwards for  $\gamma > 90^{\circ}$ , which explains the intensity bump in the curves that moves between  $0^{\circ}$  and  $90^{\circ}$ .

One can expect no negative polarization for the mentioned extreme cases, where single scattering dominates, since single cubes with the given complex refractive index and size parameter are definitely not able to bring out negative polarization. However, full wave simulations clearly point out the appearance of negative polarization for  $\gamma$  between 60° and 90° with a maximum of 4%. Further incrementing of  $\gamma$  results in strong enhancing negative polarization with a maximum of 19.5% for the range from 90° to 120° and 13% for the next one from 120° to 150° (see both sequences 4 and 5 of figure 5.6). The inversion angles of the polarization for these two ranges are 173° and 156°, respectively. Finally, as seen in the last range from 150° to 180°, sequence 6 in figure 5.6, the negative polarization vanishes again. Hence, these results demonstrate that coherent double reflection between the neighbored particles at angles, where single reflection does not dominate, is in a direct relationship for generating negative polarization. On one hand, configured two cubic structures that produce negative polarization mostly do not deliver intensity surge, where on the other hand, the ones with higher intensity surge correspond with very low or no polarization.



Figure 5.5: Intensity curves in logarithmic scale for systems of two cubes averaged over angle  $\gamma$  in six bins from 0° to 180°.



Figure 5.6: Linear polarization curves for systems of two cubes averaged over angle  $\gamma$  in six bins from 0° to 180°.

#### Chapter 5. Simulation results

After averaging over all the angles  $\gamma$  from the six sequences considered above, the normalized intensity and the linear polarization are displayed in figures 5.7a, 5.7b, respectively. Undoubtedly, negative polarization does not hold on due to the dominance of single scattering from cubes having very large and very small  $\gamma$ . This means that negative polarization can be produced when specific slope distribution of the reflecting faces take place. Otherwise, it is suppressed by large contribution of single scattering. In order to switch off the effect of the angle  $\gamma$  between two facets, a geometry with two spheres has been checked. This structure contains all possible angles  $\gamma$  between the spheres facets.



Figure 5.7: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization computed for systems of two cubes averaged over angle  $\gamma$  from 0° to 180°.

#### 5.3 Structures of two spheres

In order to study further influencing factors on the negative polarization, this effect of facets orientation has been suppressed in this section. This can be realized, when having two scatterers that build all possible orientations of their surface elements. A suitable structure that meets this condition is two identical faceted spheres as they comprise all angles  $\gamma$  ranging from 0° to 180° between their facets that build their approximated geometry. As in the case of two cubes,  $\gamma$  is constructed between two facing surface elements, each of them belongs to one sphere. Thus, all angles  $\gamma$  that have been studied for all configurations of the cubic structures are combined together in just one structure of two faceted spheres. Both spheres have the same radius. Figures 5.8a and 5.8b illustrate, respectively, the considered faceted spheres with minimum distance smaller than the wavelength of the

incident light and maximum distance that is equivalent to the diameter of the considered spheres.



Figure 5.8: Two spherical particles with minimum separation between them that is much smaller than the wavelength of the incident light in (a) and a separation of one diameter, i.e., a size comparable to one sphere as a maximum distance between them in (b).

Thereafter, the influence of slightly changing the separation between the two spheres is analyzed. Unusually, the outcome of the gradual increasing of the spheres separations in steps around 11% of the wavelength of incident light is a flip of polarization between negative polarization and positive one at the backscattering branch as can be seen in figure 5.9b. The same behavior is also obtained for larger separations of the scale of the spheres radius and diameter as figures 5.10 and 5.11b display, respectively. However, this is associated with decreased amplitude of the negative polarization and positive one. In order to focus on this effect, figures 5.12, 5.13 and 5.14 plot intensity and polarization near the backscattering range of these three studied cases for the separations: minimum, one radius and one diameter distance, respectively. The scale of the axes is uniform to allow direct comparison. Correspondingly, the peaks of negative polarization and positive one also move to backscattering range while the separation gets larger. This can be explained by the reduced contribution of the double scattering as a result of increasing the distance between both spheres. The number of oscillations at backscattering is also growing with larger separations (see figures 5.12b, 5.13b and 5.14b) because of the interference of double scattering. The minima of the normalized intensity near backscattering in figures 5.12a, 5.13a and 5.14a correlate with the minima and maxima of the polarization flip and shift as well to the right hand side with increased number of oscillations as a consequence of growing separation.



Figure 5.9: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for two faceted spheres that have size parameter kR = 30 with gradually growing distances between them starting from one much smaller that the wavelength of incident light. The distances from 1 to 7 represent slightly increased separation with steps around 11% of this wavelength for the corresponding separation.



Figure 5.10: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for two faceted spheres that have size parameter kR = 30 with gradually growing distances between them starting from one equivalent to the sphere radius. The distances from 1 to 6 represent slightly increased separation between spheres with steps around 11% of the illumination wavelength for the corresponding separation.



Figure 5.11: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for two faceted spheres that have size parameter kR = 30with gradually growing distances between them starting from one equivalent to the sphere diameter. The distances from 1 to 6 represent slightly increased separation with steps around 11% of the illumination wavelength for the corresponding separation



Figure 5.12: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for two faceted spheres that have size parameter kR = 30 with gradually growing distances between them starting from one much smaller that the wavelength of incident light. The distances from 1 to 7 represent slightly increased separation with steps around 11% of this wavelength for the corresponding separation.



Figure 5.13: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for two faceted spheres that have size parameter kR = 30 with gradually growing distances between them starting from one equivalent to the sphere radius. The distances from 1 to 6 represent slightly increased separation between spheres with steps around 11% of the illumination wavelength for the corresponding separation.



Figure 5.14: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for two faceted spheres that have size parameter kR = 30 with gradually growing distances between them starting from one equivalent to the sphere diameter. The distances from 1 to 6 represent slightly increased separation with steps around 11% of the illumination wavelength for the corresponding separation.

This polarization flip is a typical interference pattern that depends on distance changing between scatterers, as an interference base. One can see this in the frequency of oscillation in the polarization plots. To check if the same flipping behavior can be detected for other size parameters of the same structures, two close absorbing spheres  $(Im\{m\} = 0.3)$ with different size parameters are simulated with equidistantly distance variation. Figures 5.15 and 5.16 display the normalized intensity and the linear polarization of two spherical structures with size parameters kR = 24 and kR = 12, respectively.



Figure 5.15: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) computed for two faceted spheres that have size parameter kR = 24 with slightly growing separations starting from one much smaller that the wavelength of incident light. The distances from 1 to 8 represent slightly increased separation between spheres with steps around 11% of the wavelength.

#### The distance variation



Figure 5.16: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for two faceted spheres that have size parameter kR = 12 with gradually growing distances starting from one much smaller that the wavelength of incident light. The distances from 1 to 8 represent slightly increased separation between spheres with steps around 11% of the illumination wavelength for the corresponding separation

The polarization flip in both selected cases can be clearly observed, whereas the symmetry of the flipping here (see figures 5.15d and 5.16d) is broken in comparison with the polarization curve illustrated in figure 5.12b. This symmetry is broken in two distinct

ways because of two different reasons. The first one comes out because the amplitudes of the negative polarization curves are higher than the positive polarization ones at the backscattering as can be seen in figure 5.15d. While the second one as figure 5.16d shows, is due to having more curves of negative polarization than positive one at the backscattering, in spite of having equidistant steps for the separation between the two spheres. Accordingly, all these single curves, that have been taken into account, display the effects of having more curves with negative polarization over the positive polarization and having more curves with negative polarization than positive one. Both will contribute to the appearance of the negative polarization after averaging. As well, the amplitude of the polarization flip gets smaller and wider, when the size parameter of the spherical structures decreased.

Averaging the normalized intensity and the linear polarization over about 120 steps from minimum distance, i.e., nearly touching spheres to the distance of one sphere diameter delivers negative polarization with a maximum of 1.9% with an inverse angle about 172° as figure 5.18 shows. Yet, an additional sphere in the structure, as displayed in figure 5.17, results in raising the negative polarization to a maximum of 3.4% (see figure 5.18).



Figure 5.17: Three spherical particles with minimum distance in (a) and maximum distance in (b). The maximum distance here is relatively smaller than it is in the case of two spheres because of the relatively expensive computational efforts due to the huge size of the simulation domain that can result from larger separations.

These results comprehend as well with the increased negative polarization when adding a third particle for a structure consists of two irregular particles as shown in figure 5.2. Thus, it is established that while double scattering is not sufficiently strong for producing negative polarization for structures that consist of two cubes after averaging over all angles between them, it still has an effect on structures with spheres.



Figure 5.18: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) averaged over all computed separations for two and three faceted spheres.

Interestingly, the studied structure with three spheres (figure 5.17b) also delivers polarization flip when the separation is varied. The normalized intensity and linear polarization curves gained from six single simulations of three spheres are presented in figure 5.19. These curves belong to the spherical structures with separations starting from minimum distance much smaller than the wavelengths of the incident light (figure 5.17b) to larger distances with steps around 11% of this wavelength. Figure 5.19d provides a good understanding of high negative polarization that dominates in the averaged curve in figure 5.18d as all curves of the linear polarization between 170° and 180° lie mostly down to the zero axes of the polarization. This can be interpreted as a shifting of oscillations at the backscattering angles to the negative side of polarization after adding the third sphere in comparison to the case of two spheres.



Figure 5.19: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for three faceted spheres that lie on one line and have size parameter kR = 30 with gradually growing distances much smaller than the wavelength of incident light. The distances from 1 to 6 represent slightly increased separation between spheres with steps around 11% of the illumination wavelength for the corresponding separation.

Polarization flip here gets less symmetrical and strongly narrower starting from about
#### Chapter 5. Simulation results

 $175^{\circ}$ , where it begins near  $170^{\circ}$  for the case of two spheres as figure 5.12b shows. In addition, that the positive polarization branch from  $0^{\circ}$  to  $126^{\circ}$  do not get much influenced by having a third sphere. This can be seen in figure 5.18b. The scattering angle curves of three-sphere structures are averaged over 23 simulations. The reason is the heavy calculations for larger separations between the spheres of such structures. However, this average is acceptable, as this work focuses on densely packed particles, which is achieved by relatively small separations.

Spherical shapes are perfect symmetric geometries and the angles constructed between two scatterers facets are uniformly distributed. Henceforward, bringing in nonsphericity considering ellipsoidal constituents that can describe a transient case between irregular particles and spherical ones. In order to better understand the irregular particles, some irregularities, or particularly, some non-sphericity have been introduced to the spheres composing ellipsoids. This helps to interpret the influence of the angle  $\gamma$  as well as the separation distance between the two particles.

### 5.4 Structures of two ellipsoids

In this section, the sensibility of negative polarization to the particle shape or the angles  $\gamma$  constructed between the facets of two scatterers is considered. The basic structure here is binary spheres that have the same size (figure 5.8). It is used to produce binary ellipsoids with different aspect ratios. 10% stretching and squeezing of spheres diameter along y and z axes yield the ellipsoidal structures with the aspect ratios (1 : 0.9 : 1, 1 : 1.1 : 1, 1 : 1 : 0.9 and 1 : 1 : 1.1). The ellipsoids have absorbing material with refractive index m = 1.5 + i0.3. The results of the simulations are averaged over the distance between both particles starting from very small distance, much smaller than the wavelength of incident light, to a maximum distance of approximately one sphere diameter.

Figure 5.20c shows that the normalized intensity in the backscattering range increases for ellipsoidal structures from smaller aspect ratios to larger ones. This is an expected result because of the increased size parameter of the structure, which delivers more backscattering. The intensity and polarization curves of the basic two spheres are also plotted in figure 5.20 to compare the curves of ellipsoidal structures with them. It is also obtained that the normalized intensity gets differently influenced when increasing the aspect ratio in y and z direction, e.g., for 1.0:1.1:1.0 and 1.0:1.0:1.1, respectively. The structure with 10% expanded aspect ratio in y direction delivers higher intensity than the one with 10% expanded aspect ratio in z direction. The reason is that expanding the structure in y direction increases the interaction surface area with the direct incident light, which causes higher reflection. Hence, more double scattering is obtained, which explains getting higher negative polarization, correspondingly, in figure 5.20d. On one hand, the inversion angle does not change remarkably for aspect ratio variation in y direction, which

lies around  $172^{\circ}$ . On the other hand, for aspect ratio variation in z direction, the inversion angle decreases from  $175^{\circ}$  for the ellipsoids with aspect ratio 1:1:0.9 to  $169^{\circ}$  for the ones with 1:1:1.1. This is associated with growing degree of negative polarization from 1.2% to 2% in both cases, respectively. This means that negative polarization is very sensitive to the structure shape and the orientations of its facets.



Figure 5.20: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) for two ellipsoids with different aspect ratios. The curves are averaged over equidistant 120 separations between both scatterers with range from minimum distance much smaller than the wavelength of incident light and maximum equivalent to one sphere diameter.

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For getting more details, geometries comprising two ellipsoids that are stretched in y-direction are studied with varying the aspect ratios along the z-axis with 10% step variation. Figure 5.21 shows the structures that have aspect ratios from 1 : 1.5 : 0.4 to 1 : 1.5 : 1.1.



Figure 5.21: Two ellipsoidal particles (a) to (h) with minimum distance much smaller than the wavelength of incident light with 10% increased aspect ratio in z-axis for each structure starting from 1: 1.5: 0.4 to 1: 1.5: 1.1.

Figure 5.22a and 5.22b show the normalized intensity and polarization, respectively for different aspect ratio configurations. Each is averaged over around 100 separations ranging from minimum distance much smaller than the wavelength of the incident light to the maximum separation. The last corresponds to one same sized ellipsoid with the same orientation of both scatterers. As seen in Figure 5.22d, which is a zoom in of 5.22b, the structures show the existence of negative polarization (maximum of 2.3%), positive polarization (maximum of 1%) as a result of changing the distribution of angles  $\gamma$  between scatterers faces. This is a further confirmation of the effect of the angle of orientation between the surfaces of two scatterers in producing negative polarization.



Figure 5.22: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) averaged over 100 separations for binary ellipsoids with different aspect ratios from from 1 : 1.5 : 0.4 to 1 : 1.5 : 1.1.

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Unexpectedly, in figure 5.22c, the intensity surge does not seem to correlate with the negative polarization in figure 5.22d, it is rather as a consequence of the geometry of the ellipsoids themselves and their aspect ratios. It can be inferred from the normalized intensities that the intensity surge increases monotonously as the aspect ratio along z-axis reduces, which points to an increased contribution of single scattering in the backscattering direction. This implies that the intensity surge seems to be characterized more by the shape of the particles and not correlating with negative polarization. Moreover, averaging the normalized intensity and the linear polarization over all aspect ratios from 1: 1.5: 0.4 to 1: 1.5: 1.1 reveals a clear minimal negative polarization, as figure 5.23 represents.



Figure 5.23: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) averaged over all binary ellipsoids with aspect ratios from 1: 1.5: 0.4 to 1: 1.5: 1.1.

The negative polarization here, which is an average over hundreds of computations, starts at an inversion angle around 173° and amounts to a maximum of 0.6%. Accordingly, this can give an explanation of the weak negative polarization observed for two irregular particles. As a consequence of this result, for producing the negative polarization by GRF particles, three factors are involved. The effect of their random irregular shapes, the orientations of their facets and the separation between them. This suggests that the negative polarization obtained from just two particles is not always sufficiently strong to show up the averaged results. However, double scattering shows responsibility for producing the negative polarization.

Studying the existence of the polarization flip behavior corresponding to the distance variation between scatterers for ellipsoidal structures can be a forward movement to examine the generality of this flip for non-spherical structures. At this point figures 5.24, 5.25, 5.26, and 5.27 show the scattering angle dependencies of normalized intensity and linear polarization computed for the first minimum separations between two ellipsoids with the aspect ratios: 1:1.5:0.4, 1:1.5:0.6, 1:1.5:0.8, and 1:1.5:1.1, respectively. Only simulations of the first few minimum separations are considered because of two reasons. First, powder structures in nature are mostly densely packed, i.e., powder particles have minimum distances between them or touch each other. Second, as in the case of two spheres, when the particles are too close, the amplitude of polarization flip acquires its maximum. Hence, allowing for better comparison of the results. In the purpose of direct comparison, all these plots have the same scales. As well, their zoomed in polarization curves (figures 5.24d, 5.25d, 5.26d, and 5.27d) have a scale comparable with figure 5.12b that belongs to binary spheres.

All the chosen ellipsoidal structures exhibit polarization flip at backscattering range. The minima and maxima of this flip take place in the four considered cases mostly around scattering angel 176°. However, in an asymmetrical way that will be discussed here. The first two ellipsoids that have the aspect ratio 1 : 1.5 : 0.4 deliver the least amplitude of polarization flip between -9.7% and 4.8%. The explanation for this is, the smaller the aspect ration in z-direction is, the smaller interaction between scatterers surfaces is happening, and consequently, the smaller is the contribution of double scattering that should be responsible for polarization flipping at backscattering range. In particular, such a relative smaller aspect ratio in z-direction means less convexity of the ellipsoidal surface in front of the incident light. Thus, more light get scattered back. This explains the relatively higher intensity at backscattering in figure 5.24a in comparison with the intensities of the other considered aspect ratios in figures 5.25a, 5.26a and 5.27a, which get decreased at backscattering with growing aspect ratio in z-direction. The results for structures with aspect ratio 1: 1.5: 0.6 (see figure 5.25d) have more amplitude of polarization flip than the previous one. It amounts between a minimum of -13% and a maximum of 15%.



Figure 5.24: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for two faceted ellipsoids with aspect ratio 1: 1.5: 0.4 that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 6 represent slightly increasing separation between ellipsoids with steps around 11% of the illumination wavelength.



Figure 5.25: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for two faceted ellipsoids with aspect ratio 1: 1.5: 0.6 that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 6 represent slightly increasing separation between ellipsoids with steps around 11% of the illumination wavelength.

The geometry with aspect ratio 1 : 1.5 : 0.8 (figure 5.26d) shows further increased amplitude of polarization flip between -20% and 30%. The positive polarization curves dominates here, where in contrast, for the aspect ratio 1 : 1.5 : 1.1 as figure 5.27d displays, the polarization in the curves on the negative side at backscattering has higher amplitudes than ones on the other side. Its amplitudes amounts to a minimum of -30%

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and a maximum of 27%. That is, both these aspect ratios 1 : 1.5 : 0.8 and 1 : 1.5 : 1.1 establish that the balance between the negative and the positive polarization curves at backscattering get changed, when varying the particle geometry.



Figure 5.26: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for two faceted ellipsoids with aspect ratio 1:1.5:0.8 that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 6 represent slightly increasing separation between ellipsoids with steps around 11% of the illumination wavelength.



Figure 5.27: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for two faceted ellipsoids with aspect ratio 1:1.5:1.1 that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 6 represent slightly increasing separation between ellipsoids with steps around 11% of the illumination wavelength.

It is clear now, that when having scatterers with the same size parameter and material, that the intensity and polarization at backscattering depend strongly on the scatterers shapes and the separation between them. Subsequently, the packing density of particles should play a big role as well. It was concluded in this section that the lower intensity near backscattering correlates with higher amplitude of polarization flip, and vice versa.

## 5.5 Polarization flip obtained by irregular particles

Double scattering has a significant influence on the negative polarization for cubes, spheres and ellipsoids. It is interesting to explore if the polarization flip at backscattering branch obtained by structures of regular shapes for separation variation can also be produced by irregular shapes. To answer this question, arbitrary chosen structures of two irregular particles that are randomly oriented with distance variation between them have been studied. The scale of separation here is much smaller than the wavelength of the incident light and it grows to distances equivalent to the size of one particle in 120 steps. Calculations have been performed for two different sets of these structures, i.e., two random cases for double particles. Figures 5.28 and 5.29 show both considered structures with minimum and maximum distance between scatterers.



Figure 5.28: Set 1 of arbitrary chosen two irregular GRF particles that posses a size parameter kR = 30 with minimum distance between them much smaller than the wavelength of the incident light in (a) and maximum separation comparable to the size of one particle in (b)



Figure 5.29: Set 2 of arbitrary chosen two irregular GRF particles that posses a size parameter kR = 30 with minimum distance between them much smaller than the wavelength of the incident light in (a) and maximum separation comparable to the size of one particle in (b)

#### 5.5 POLARIZATION FLIP OBTAINED BY IRREGULAR PARTICLES

The linear polarization curves of both instances demonstrated in the following plots confirm that the polarization flip is still observed in both sets of two irregular particles, especially, for very small separations as can be seen in figures 5.30b, 5.36b and their zoomed in plots 5.33b and 5.39b, respectively. This proves that the negative polarization is sensitive to particles separation, and consequently, to the density of particles agglomerates for powder-like surfaces. However, the symmetry of the negative polarization is broken in comparison to regular shapes, which is an expected result because of the random irregular shapes. Additionally, all polarization curves for separations of half size parameter of first set (see figures 5.31b, 5.34b) and second set (figures 5.37b and 5.40b) reveal that increasing the separation between particles results in decreasing the amplitude of negative and positive polarization flip at backscattering because light interaction between particles get reduced. Therefore, the contribution of double scattering, which is responsible for the negative polarization here, becomes smaller. The same is also valid for one size parameter separation as figures 5.32b, 5.35b of the first set and 5.38b 5.41b of the second one show.

Interestingly, figures 5.31b and 5.34b show that the polarization flip does not occur only at the last oscillation near backscattering, as it was obtained for spheres. It appears rather for both previous oscillations between scattering angles 165° and 175° with increased amplitudes for decreased angles. This depends on the geometries of the investigated random irregular particles, their separation and orientation.

The intensity curves of the first binary particle set in figures 5.30a, 5.31a and 5.32a and their zoomed in plots (figures 5.33a, 5.34a and 5.35a) show the result of increased number of oscillations with growing separation. The same is also obtained in the second set (figures 5.36a, 5.37a and 5.38a and their zoomed in plots (figures 5.39a, 5.40a and 5.41a). This is the same observation like in the case of regular shapes because of increased interference due to increased distances between scatterers. Furthermore, the maxima of the last oscillation of intensity curves correlate with the minima and maxima of the polarization flip at backscattering. This is in agreement with the results of regular shapes as well. Remarkably, the normalized intensity in figure 5.34a for half size parameter distance is higher than both intensities of minimum distance and one size parameter distance as can be seen in figures 5.33a and 5.35a, respectively. The reason is the shadowing effect when the particles are close to each other. In addition, the contribution of electromagnetic waves that are double scattered in the backscattering range for half size parameter distance is higher in comparison with cases that have larger separations. However, for further growing of separation between particles, the light interaction between both particles decreases, which explains the lower intensity for the maximum considered separation between particles in figure 5.35a. It is essential to mention here, that the geometry of the considered shapes play a decisive role in the intensity of the entire system.



Figure 5.30: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for the first set of two GRF particles that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 4 represent slightly increased separation between both particles with steps around 11% of the wavelength.



Figure 5.31: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for the first set of two GRF particles that have size parameter kR = 30 with gradually growing distances starting from one comparable to half size of one particle. The distances from 1 to 7 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.32: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for the first set of two GRF particles that have size parameter kR = 30 with gradually growing distances starting from one comparable to the size of one particle. The distances from 1 to 7 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.33: Scattering angle curves of (a) normalized intensity and (b) linear polarization near backscattering branch calculated for the first set of two GRF particles that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 4 represent slightly increased separation between both particles with steps around 11% of the wavelength.



Figure 5.34: Scattering angle curves of (a) normalized intensity and (b) linear polarization near backscattering branch calculated for the first set of two GRF particles that have size parameter kR = 30 with gradually growing distances starting from one comparable to half size of one particle. The distances from 1 to 7 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.35: Scattering angle curves of (a) normalized intensity and (b) linear polarization near backscattering branch calculated for the first set of two GRF particles that have size parameter kR = 30 with gradually growing distances starting from one comparable to the size of one particle. The distances from 1 to 7 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.36: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for the second set of two GRF particles that have size parameter kR = 30 with gradually growing distances comparable to the size of one particle. The distances from 1 to 6 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.37: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for the second set of two GRF particles that have size parameter kR = 30 with gradually growing distances comparable with half size parameter. The distances from 1 to 7 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.38: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization calculated for the second set of two GRF particles that have size parameter kR = 30 with gradually growing distances comparable to the size of one particle. The distances from 1 to 6 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.39: Scattering angle curves of (a) normalized intensity and (b) linear polarization near backscattering branch calculated for the second set of two GRF particles that have size parameter kR = 30 with gradually growing distances comparable to the size of one particle. The distances from 1 to 6 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.40: Scattering angle curves of (a) normalized intensity and (b) linear polarization near backscattering branch calculated for the second set of two GRF particles that have size parameter kR = 30 with gradually growing distances comparable with half size parameter. The distances from 1 to 7 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.



Figure 5.41: Scattering angle curves of (a) normalized intensity and (b) linear polarization near backscattering branch calculated for the second set of two GRF particles that have size parameter kR = 30 with gradually growing distances comparable to the size of one particle. The distances from 1 to 6 represent slightly increased separation between both particles with steps around 11% of the wavelength of incident light.

# 5.6 Confirmation of the effect of double scattering on polarization at backscattering

Initially, for the considered high absorption  $(Im\{m\} = 0.3)$ , the negative polarization can not be produced by scattering from single particles. It appears for structures consisting of double particles at least. In this section, the reflecting area of the structures is increased, but mostly preserve the distribution of angles  $\gamma$ . This has been done in two procedures. The first one is direct comparison between two binary structures, namely, binary spheres and binary ellipsoids. The ellipsoids are gained by stretching the spheres in *y*-direction 1.5 times. Hence, they have the aspect ratio 1: 1.5: 1 and size parameter kR = 45. The second one is increasing the size of entire system making the number of spheres larger. Here, monolayers of five and seven spheres are studied.

Figure 5.42 illustrates the first case of binary structures of spheres and ellipsoids. The opposite surfaces of ellipsoids are larger than the ones of spheres. Thus, higher double scattering contribution according to rising the faces area, where light interacts between both scatterers, is achieved.



Figure 5.42: Structures of two faceted spheres and ellipsoids in (a) and (b), respectively, with minimum separation between them.

The ellipsoids are formed by of extending the same studied spheres only in y-direction, which is the perpendicular direction to the incident light. Figure 5.43 and its zoom at backscattering angles figure 5.44 display the scattering angle curves of the normalized intensity and the linear polarization of the considered spherical and ellipsoidal shapes. These plots have the same scale in order to compare the curves with each other. The intensity at the backscattering branch for ellipsoids (figures 5.43c and 5.44c) shows enhancement in comparison to the one of spheres (figures 5.43a and 5.44a). This occurs because the ellipsoids have larger surface areas that lie in front of the incident wave and

#### 5.6 Confirmation of the effect of double scattering on polarization at backscattering

scatter more light back.



Figure 5.43: Scattering angle curves of normalized intensity in logarithmic scale of (a) two faceted spheres and (c) two faceted ellipsoids that have aspect ratio 1 : 1.5 : 1 and (b), (d) linear polarization near backscattering branch calculated for the same order with gradually increasing distances starting from one much smaller than the wavelength of the incident light. The distances from 1 to 7 represent slightly increased separation between both regular particles with steps around 11% of the wavelength.



Figure 5.44: Zoomed in scattering angle curves of (a), (c) normalized intensity of two faceted spheres and two faceted ellipsoids (aspect ratio 1 : 1.5 : 1), respectively, and (b), (d) linear polarization near backscattering branch calculated for the same both structures with the same order with gradually increasing distances starting from one much smaller than the wavelength of the incident light. The distances from 1 to 7 represent slightly increased separation between both regular particles with steps around 11% of the wavelength.

Now, the polarization curves are considered in figures 5.43b and 5.43d, especially at the backscattering range, which is zoomed in 5.44b and 5.44d. Importantly, for the case of two spheres, the maximum amplitude of the polarization flip amounts to 29% for the negative and 28% for the positive one, where for ellipsoids, this amplitude is clearly

higher. It gets a value around 31% for negative and 37% for positive polarization. Hence, increasing the double scattering that is achieved throw extending the spheres to ellipsoids in the horizontal direction, which is responsible for rising the degree of polarization for the corresponding separation.

The second procedure, which is increasing the number of scatterers, is discussed here. It was shown in chapter 5.1 that increasing the number of particles demonstrated growing of the degree of negative polarization at backscattering. The same happens when adding a third sphere to the structures of double spheres. Thus, systems with larger numbers of particles have been studied. A good choice here is cluster of spherical shapes, as irregular constituents have complex topologies and deliver hardly interpretable single (not-averaged) curves. Structures of five and seven spheres, as figure 5.45 displays, are investigated. The size parameter of each sphere is 30 and their material is absorbing with refractive index m = 1.5 + i0.3. The polarization flip obtained through slightly increasing of separations from minimum distances much smaller than the wavelength of incident light with equidistant steps of 11% of wavelength.



Figure 5.45: A cluster of (a) five and (b) seven faceted spherical particles in with minimum separations between them.

Although dealing with spheres looks from the first sight not enough for theoretical modeling of natural powder, the following plots (figures 5.46 and 5.47) give a concrete argument that increasing the number of scatterers, increases in turn the degree of the positive and negative polarization at backscattering. The reason for that is the increasing of double scattering contribution. Polarization flipping behavior (see figures 5.46d and 5.47d) is still observed at backscattering with minimum of -52% at 177° and maximum of 56% at 177.5° for five spheres. The degree of polarization flip for the seven scatterers amounts to a minimum of -62% at 176.8° and maximum of 79% at 177°. Nevertheless, for 5 spheres case, it seems more symmetric than 7 spheres case. One can say, this is the result of accumulating all interactions between spheres, i.e., superposition of double scattering between each two particles.

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The intensity at backscattering gets lower for structures of 5 spheres in comparison with 7 ones as figures 5.46c and 5.47c, which have the same scale, display. This is because of the coherent backscattering enhancement associated with increasing the number of scatterers.



Figure 5.46: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for five faceted spheres that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 7 represent slightly increased separation between both ellipsoids with steps around 11% of the wavelength.



Figure 5.47: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for seven faceted spheres that have size parameter kR = 30 with gradually growing distances starting from one much smaller than the wavelength of incident light. The distances from 1 to 5 represent slightly increased separation between both ellipsoids with steps around 11% of the wavelength.

## 5.7 The role of refractive index m

For studying the influence of the real part of refractive index m on polarization, twosphere structures are first investigated with the same absorbing material  $Im\{m\} = 0.3$ and different  $Re\{m\}$ . Again, the polarization flip obtained from variation of separation

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between both spheres starting from minimum distance is considered. Figure 5.48 displays the normalized intensity and negative polarization at backscattering for two values of the real part of refractive index  $Re\{m\} = 1.5$  and  $Re\{m\} = 1.8$ . The polarization plots (see figures 5.48b and 5.48d) show an influence on the polarization amplitudes at backscattering.



Figure 5.48: Zoomed in scattering angle curves of (a), (c) normalized intensity calculated for of two spherical structures with two distinct real part of refractive index, namely,  $Re\{m\} = 1.5$  and  $Re\{m\} = 1.8$ , respectively and (b), (d) linear polarization near backscattering branch calculated for the same both refractive indices, respectively. The distances from 1 to 7 represent slightly increased separation between both scatterers starting from one much smaller than the wavelength of incident light with steps around 11% of the wavelength for the corresponding separation.

The intensity gets higher with increasing  $Re\{m\}$  from 1.5 to 1.8 due to Fresnel reflection. This can be seen in both figures 5.48a and 5.48c, when comparing the curves with each other as they have the same scale. For m = 1.5 + i0.3 the minimum polarization degree is -29% and the maximum one is 28%, where both increase with increasing the real part of m to 1.8. Here, the polarization degree amounts to a minimum of -30% and a maximum of 30%.

It is interesting to study now, if the real part of refractive index can impact the negative polarization for clusters of irregular particles. Sufficient structure for this target is a monolayer of ten irregular particles. An example of this structure is displayed in figure 4.2 in the model description section 4.1. Clusters consisting of more particles like 50 or 100 do not produce much changes in the negative polarization at backscattering [115]. Thus, heavy computational effort is saved using monolayers consisting of ten irregular particles instead of simulating multiple layers with tens or hundreds of particles. One hundred simulations with these structures with variation of the real part of refractive index have been done.

The refractive index of the monolayer of irregular particles has the same imaginary part but different real parts (m = 1.3 + i0.3, m = 1.5 + i0.3 and m = 1.8 + i0.3). The intensity curves (see figures 5.49a and 5.49c) show similar profiles at backscattering range with increased amplitudes as a result of rising the real part of refractive index, which is expected. The curves display increased negative polarization at backscattering up to 0.1% for each increase of  $Re\{m\}$  as figure 5.49d illustrates. The degree of negative polarization for m = 1.3 + i0.3 is 1.9%, where the next one for m = 1.5 + i0.3 amounts to 2% and the last for m = 1.8 + i0.3 makes 2.1%. Another effect here is that the positive polarization at intermediate angles shifts to the left hand side with increased  $Re\{m\}$ . Figure 5.49b shows this. As well, the maximum of positive polarization increases for growing the real part of refractive index. It amounts to 85.8% for  $Re\{m\} = 1.3$ . For  $Re\{m\} = 1.5$  it grows to 86.7% and it gets its maximum for  $Re\{m\} = 1.8$  at 87.2%. This can also be seen in figure 5.49b. Changing  $Re\{m\}$  of the scattering object influences Brewster's angle of its single scattering, which impacts the scattered light. One can say that Brewster's angle has an effect on the negative polarization.

The imaginary part of the refractive index  $Im\{m\}$  that describes the absorption is a critical parameter for light scattering in general. It also influences the opposition phenomena strongly. It affects the linear negative polarization so that single absorbing particles do not produce it any more. This is, in fact, the opposite case for non-absorbing ones that deliver negative polarization at backscattering. In order to study absorption theoretically, one needs to model the variation of the imaginary part of the refractive index  $Im\{m\}$  to see how it affects the intensity and the linear polarization. The goal here is to figure out, after gradual increasing of absorption for single particles starting from transparent ones, when the negative polarization starts to disappear.



Figure 5.49: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for a monolayer of ten random irregular particles with three different real parts of refractive index, namely, 1.3, 1.5 and 1.8. The size parameter of each constituent is kR = 30. The curves are averaged over 100 samples.

It is interesting to find the value of  $Im\{m\}$  for which the negative polarization of single particles vanishes to use this value for cluster of particles. This requires choosing different values for  $Im\{m\}$  between 0 and 0.3 which represents high absorption. As averaging over hundreds of heavy numerical simulations for each value of  $Im\{m\}$  is computationally expensive, it makes sense to probe a few calculations for simple regular shapes to get some approximation for these values. After that, the results of regular shapes will be used for computations of single irregular particles. For this reason, a set of twelve ellipsoids that possess different aspect ratios have been investigated. Their aspect ratios vary from 1 : 1.5 : 0.4 to 1 : 1.5 : 1.5 with variation of 0.1 steps on the z axes and the size parameter is kR = 30. For calculations performed for this set of ellipsoids arbitrary values of  $Im\{m\}$  are chosen between 0 and 1 as the plots in figure 5.50 show. It is worthy to mention here, that averaging over twelve single curves of ellipsoidal structures with different aspect ratio is not enough for studying single scattering of different absorbing materials. Even-though it gives a rough estimation about the effect of the imaginary part of the refractive index on the normalized intensity and linear polarization as one can see in figure 5.50. Each curve here is the result of averaging over only 12 curves of the single ellipsoids. The polarization curves in 5.50b illustrate that the influence of absorption is significant, especially in the interval between  $Im\{m\} = 0.01$  and  $Im\{m\} = 0.1$ , where the the polarization curves strongly change their pattern. At this point this range of  $Im\{m\}$  between 0.01 and 0.1 is interesting to investigate for light scattering from single irregular particles.



Figure 5.50: Scattering angle curves of (a) normalized intensity in logarithmic scale and (b) linear polarization computed for single ellipsoids with growing absorption starting from transparent particles  $(Im\{m\} = 0)$  to relatively high absorption  $(Im\{m\} = 0.1)$ . Each curve is averaged over 12 different aspect ratios between 1: 1.5: 0.4 and 1: 1.5: 1.5 with variation of 0.1 step on the z axes. that have size parameter kR = 30, where the negative polarization disappears.

Accordingly, single irregular particles with size parameter kR = 30 have been considered using the obtained  $Im\{m\}$  values as figure 5.51 demonstrates. Each curve is an average over more than 200 computations of different single particle modifications. In general, light scattered by non-absorbing single particles delivers negative polarization

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and an intensity surge. The polarization for intermediate scattering angles moves in the positive direction with increased absorption 5.51b, where at backscattering the case is different. Transparent single particles produce negative polarization that amounts to 1.7% with inversion angle 170° as figure 5.51d displays. Interestingly, when increasing absorption  $Im\{m\}$  to 0.01, the negative polarization gets enhanced and it shows a maximum of 2% at 169°. After this point consequent increasing of the absorption gradually decreases the negative polarization till it vanishes for the refractive index m = 1.5 + i0.06, where the curve of the linear polarization takes its well known character of Fresnel polarization. This means that the relatively high absorption of the single irregular particles blocks the single scattering contribution to the negative polarization completely for  $Im\{m\} = 0.06$ . This shows, when the particles are transparent the main source of negative polarization in this system is single scattering until they become non-transparent.

In clusters of random irregular particles, there are single and multiple scattering, but for single particles, one can also define internal scattering. For single particles, single external reflection and multiple internal scattering can be considered. In fact, as long as particles are transparent, strong single external reflection and multiple internal scattering exist in the system. The roles of these single and multiple scattering are different as single scattering is the source of negative polarization, but in contrast, the internal multiple scattering is a depolarization factor. Thus, reducing the contribution of positive and negative polarization. In other words, in the purpose of analyzing the curves in figure 5.51d, modifying  $Im\{m\}$  changes the balance between external single and internal multiple scattering. The result is not general but it is still interesting because it clarifies that the dependency here is not monotonous, as this multiple scattering decreases faster than the single one when rising  $Im\{m\}$ . This explains having a maximum of negative polarization at  $Im\{m\} = 0.01$ . As absorption growing reduces the contribution of internal multiple scattering, i.e., decreases the depolarization effect, and only a relative contribution of single scattering is still observed. This single scattering contribution is responsible for the negative polarization enhancement. Further increasing of the absorption decreases both external single and internal multiple scattering until negative polarization for single particles disappears. In addition, the normalized intensity and the linear polarization curves do not exhibit a relationship between negative polarization and intensity surge at backscattering. Gradual increasing of the absorption decreases the intensity and the intensity surge gets weaker until m = 1.5 + i0.1 and it increases again for m = 1.5 + i0.3as figures 5.51a and 5.51c displays.

As single scattering does not produce negative polarization for single GRF particles with absorption higher than  $Im\{m\} = 0.06$ , it is interesting to study such high absorption for monolayers of 10 irregular particles. This allows considering the contribution of double scattering to the negative polarization without the single scattering one. Therefore, two different values of  $Im\{m\}$  have been employed, namely, 0.1 and 0.3. As well, for comparison, simulations for the same structures with  $Im\{m\} = 0$  are done. The size parameter of each particle in the monolayers is kR = 30. Figure 5.52 shows the normalized intensity and linear polarization curves for these three cases. Each curve is averaged over around 300 samples. The negative polarization appears for all three cases, where in contrast, for the same considered refractive indices, only the non-absorbing single irregular particles were able to produce negative polarization at backscattering.



Figure 5.51: Scattering angle curves of (a), (c) normalized intensity and (b), (d) linear polarization calculated for single (isolated) GRF particles that have size parameter kR = 30 with growing absorption starting from transparent particles  $(Im\{m\} = 0)$  to relatively high absorption  $(Im\{m\} = 0.1)$ , where the negative polarization disappears. Each curve is averaged over more than 200 computations.

On one hand, the polarization curves in figure 5.52b show profile very close to the similar one of single particles for intermediate scattering angles. On the other hand, not

only the non-absorbing clusters of 10 particles generate negative polarization but also the absorbing ones. This is opposed to scattering by absorbing single particles, as their polarization curves starting from  $Im\{m\} = 0.06$  do not possess negative polarization at all (see figure 5.51b).



Figure 5.52: Scattering angle curves of (a), (c) normalized intensity and (b), (d) linear polarization calculated for a monolayer of ten GRF particles that have size parameter kR = 30 with three levels of absorption starting from transparent constituents ( $Im\{m\} = 0$ ) to relatively high absorption ( $Im\{m\} = 0.1$  and  $Im\{m\} = 0.3$ ), where the negative polarization appears again in contrast to single irregular particles. Each curve in this plot is averaged over around 300 samples.

Furthermore, for the case of transparent clusters, the source of negative polariza-

tion at backscattering is single scattering from the particles lying in the upper layer of the system [29]. The appearance of negative polarization for absorbing layers can be explained with interference mechanism of double scattering between the particles, as multiple scattering decreases exponentially for materials with high absorption or low albedo. In addition, it is remarkable in figure 5.52d, that non-absorbing clusters have more oscillations than the absorbing ones because of the resonances as an outcome from transparent particles of the same size. Interestingly, the degree of negative polarization grows with rising the imaginary part of refractive index as both polarization curves for absorbing clusters with m = 1.5 + i0.1 and m = 1.5 + i0.3 in figure 5.52d display. This can be interpreted as higher absorption dampens the multiple scattering non-monotonously, which decrease the depolarization. Also the inversion angle in this plot decreases with increased absorption.

## 5.8 Variation of the scatterers' size parameter

The size parameter of scattering objects influences the negative polarization. This has been found in photopolarimetric observations [9, 19, 116]. As well, it has been studied experimentally for transparent and absorbing irregular clusters of particles [12,21]. Generally, the effect of increasing the particle sizes result in increased negative polarization amplitude associated with decreasing of the inversion angle. Figure 5.53 confirms this. It shows the curves of the normalized intensity and the degree of negative polarization gained from systematic study of monolaver clusters consisting of ten densely packed irregular particles with the size parameters kr = 20 and 30. The polarization in general gets weaker with decreased sizes as the polarization curve in figure 5.53b displays for both intermediate and backscattering angles. The degree of the negative polarization makes 1.34% at the scattering angle  $172.3^{\circ}$  for particles with size parameter 30 and 0.78% for the ones with kr = 20 at 173°. The reason behind this is that when the particles are large in comparison to the wavelength of incident light Fresnel-like reflection becomes dominating in the scattering from a system. In addition, when considering the inversion angle of the polarization curve, it decreases from 167.1° to 165.8° due to growing size parameter from 20 to 30 (see figure 5.53d). This also matches with the results achieved from observational data and laboratory measurements [12, 19, 21, 116]. Chapter 5.3 shows agreement with this fact, as decreasing the sizes of two spherical structures with small distance variation delivers wider polarization flip near the backscattering with decreased amplitude (see figures 5.12b, 5.15d and 5.16d). Taking the intensity curves at the backscattering branch into account (see figures 5.53a and 5.53c) shows increasing of the intensity surge belonging to kr = 30 over kr = 20 associated with increased negative polarization. Consequently, the intensity surge of the structures of irregular particles that have size parameter 30 is narrower than the one of 20 as can be seen in figure 5.53c. This correlates with narrower negative polarization feature that can also be seen in both polarization curves as a result

#### CHAPTER 5. SIMULATION RESULTS

of increasing the scatterers' sizes regarding to the wavelength. Generally, one can say that increasing the size parameter leads to increased negative polarization and intensity surge at the backscattering range with narrower effects. This is also consistent with experimental results and approximate models. The question then arises: Does this mean that the negative polarization and intensity surge correlate with each other? The next chapter will answer this question and provide a detailed description with purposeful computations.



Figure 5.53: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for a monolayer of ten random irregular GRF particles with two different constituents size parameter, namely, kR = 20 and 30. The curves are averaged over more than 200 samples.

## 5.9 Correlation between negative polarization and intensity surge

The following figure 5.54 displays three samples of irregular constituent particles that fall down into a cylindrical domain to build the model clusters. Although all constituents are randomly oriented, it is obvious that the surface profiles can be categorized into two groups regarding to the constructed topology.



Figure 5.54: Views from the top (a, c, e) and bottom (b, d, f) of 3 distinct samples belonging to monolayer of 10 randomly oriented irregular GRF particles.

#### Chapter 5. Simulation results

The first one is represented by random topography and random distribution of heights. The second is represented by the same set of samples illuminated from the bottom side. In this case, the highest points of all particles appear on the same level as a result of deposition on a plane substrate. The motivation of this categorization is the different behavior of the same structure, when illuminating it from the top and from the bottom. At this point taking the angles of face orientations  $\gamma$ , discussed in chapters 5.2 and 5.3, into account again provides prediction of the influence of the clusters surface geometry on producing negative polarization and intensity surge. It is clear that the top side of the monolayer (figures 5.54a, 5.54c and 5.54e) allows good condition for light interaction between the neighboring particles. Consequently, this leads to higher contribution of double scattering, which is responsible for the negative polarization. In contrast, for illuminating the monolayer from the bottom side, single scattering dominates. This happens because most of the facets in front of the incident electromagnetic wave build together kind of plane-like topology perpendicular to the incidence direction (figures 5.54b, 5.54d and 5.54f). In other words, the plane areas have larger fraction than voids or corner-like structures. Hence, double scattering between the particles gets weak, which results in getting weak or even no negative polarization as a consequence. At the same time, higher light reflections at the backscattering range from these plane-like topologies are obtained, which in turn results in enhancing the intensity with increased contribution of specular reflections. This can be seen in the results of the numerical simulations from hundreds of such structures consisting of 10 uniquely shaped randomly oriented particles that are plotted in figure 5.55. Here are the curves of the normalized intensity and the degree of linear polarization from both cases, namely, illumination from the top and from the bottom of the monolayer. The negative polarization gained after illuminating the structures from the top is relatively strong and makes 1.34%. The one of bottom illumination is absent as can be seen in figure 5.55d. Whereas the intensity (figure 5.55c) shows very strong enhancement for the down side of the cluster in comparison to the upper side because of the high contribution of the specular reflection.

Typically, in the literature, there have been discussions about correlation between the negative polarization and the intensity surge. They are often observed together. However, many exceptions have been found [9]. The computations in this work, which consider realistic models, do not confirm direct or proportional correlation between both effects. They come out together when the angles  $\gamma$  between the scatterers facets allow high contribution of double scattering. In this case, negative polarization gets its maximum and the intensity surge can still exist. Additionally, when the topology of the cluster surface is more flat, double scattering conditions are not good enough and single scattering dominates for back reflections. As a result, the negative polarization gets weaker or even does not survive. Nevertheless, the intensity achieves its maximum at backscattering (see figure 5.55c).

As a conclusion, it has been found that the opposition phenomena are very sensitive to the angles  $\gamma$  built between the scatterers facets or the slope of these faces and their orientations to each other. The polarization sensitivity to the scatterers topology and composition has also been found in polarimetric observations for surfaces of planets [15]. This means generally, it is possible to create clusters or layers of irregular particles with reduced variation of slopes, which changes the balance between single and double scattering, so that negative polarization can disappear.



Figure 5.55: Scattering angle curves of normalized intensity in logarithmic (a) and linear (c) scales and degree of linear polarization (b), (d) calculated for a monolayer of ten random irregular GRF particles with two different illumination directions, namely, from top and from bottom. The constituents have the refractive index m = 1.5 + i0.3 and the size parameter kR = 30. The curves are averaged over more than 200 samples.
#### 5.10 Comparison with laboratory measurements

The linear polarization curve corresponding to monolayers of ten GRF particles (kR = 30) with absorbing material m = 1.5 + i0.3 are compared with polarization data of a sample of boron carbide powder ( $B_4C$ ) taken from the reference [21]. Figure 5.56 displays this comparison. The constituents size parameter of the experimental study is close to the one in simulations. Despite having some differences between simulations and measurements in polarization amplitudes, one can see that the inversion angles are very close to each other (between 166° and 167°). The slope of polarization between 160° to 170° and the amplitude of negative polarization vary because of the different used refractive indices, though they are absorbing. Importantly, the surface roughness and inhomogeneity of particles in addition to some distribution of their sizes in real powder can play a significant role in reducing polarization. Surface roughness depolarizes Fresnel reflection. Whereas the absorbing GRF particles used in this work have smooth surface. This can explain the difference of negative polarization between both considered cases in figure 5.56b.



Figure 5.56: Linear polarization degree in (a) and (b) for simulations of monolayer consisting of ten irregular absorbing particles and experimental data of a slab of boron carbide powder taken from figure 4b of the reference [21].

5.10 Comparison with laboratory measurements

## 6

## HighPerMeshes Project

Due to the increasing necessity for large scale simulations and the drastically growing availability of high performance computing (HPC) platforms, the domain specific language (DSL) HighPerMeshes has been developed. Thus, taking advantage of HPC systems. It is designed for application programmers from science and industry areas to implement portable parallelized iterative algorithms productively on unstructured meshes. High-PerMeshes [74–76, 117] is a collaboration project funded by BMBF (German Ministry of Education and Research) as a C++-embedded framework for heavy or large scale scientific simulations with unstructured meshes, which enables spatial flexibility and high accuracy in comparison to structured ones. The current supported numerical methods by the project include the discontinuous Galerkin method and finite element method. Utilizing parallel techniques and libraries in the software makes it very effective and performant. However, it is time consuming to learn these techniques. The HighPer-Meshes framework has the advantage of portability on heterogeneous computational architectures and super computing platforms (CPUs, GPUs and FPGAs) with efficient parallelization and scheduling in the background. Hence, there is no need to deal with porting or parallelization of the code. This increases the productivity of the developers, allowing them to concentrate on their own science and correctness of the results. HighPerMeshes supports all dimensions for 1D, 2D and 3D meshes. It provides different data structures and wrappers to fit scalar or vector fields with a lot of purposeful functionalities for numerics and related mathematical matrix vector operations. Geometrical functions used by most of the simulation methods are included in the DSL, like: GetCenter(), GetJacobian() and GetNormal(). Also topological information for the mesh is contained, for example: GetIndex(), GetIndexOfNeighberingCell() and IsElementOfBoundary(). Consequently, this offers a high abstraction level of the programming language saving time and effort for implementing, testing and debugging

#### 6.1 DGTD MAXWELL SOLVER IMPLEMENTATION IN HIGHPERMESHES

a lot of basic mathematical operations. Additionally, the framework possesses time and space loop types that are embedded efficiently in modern C++ like the following code example: ForEachEntity(use some data in a tetrahedron){ do calculations }. By means of these loop types, one can iterate over particular user chosen regions, like defining a source plane in certain position of the simulation domain for injecting the electromagnetic wave, or selecting a specific group of cells to collect the executed field values on its nodes.

A part of this thesis is the contribution to the HighPerMeshes project. The successfully accomplished tasks of this contribution are listed in the following items:

- Analyzing the DGTD method by means of the open source midg [65] and an in-house parallel DGTD code that runs on multiple CPUs [66].
- Providing an overview of DGTD, as described in chapter 3.
- Determination of the framework requirements for DGTD Maxwell solver from the user side for a compact design, useful language elements and practical operations on the mesh elements.
- Implementing field manipulation operations for representing the numerical solution on a structured grid (see figure 6.1b) from the unstructured one (see figure 6.1a). This is based on the codes described in [65, 66]. Thus, visualization with desirable user defined resolution is possible.
- Validation of the simulation results of DGTD Maxwell solver for an initial value problem in free space.
- Contribution to publications with project partners [74–76, 117].

### 6.1 DGTD Maxwell solver implementation in High-PerMeshes

In this section, the implementation of the DGTD Maxwell solver in HighPerMeshes is described and code segments are presented [74,117]. As a start point, Maxwell's equations in vacuum are implemented without material properties. This means that the numerical scheme discussed in chapter 3 (see equations 3.8 and 3.9) is simplified as follows:

$$\dot{\mathbf{E}}^{k} = \mathcal{D}^{k} \times \mathbf{H}^{k} + (\mathcal{M}^{k})^{-1} \mathcal{F}^{k} \Big( \Delta \mathbf{E} - \mathbf{\hat{n}} \cdot (\mathbf{\hat{n}} \cdot \Delta \mathbf{E}) + \mathbf{\hat{n}} \times \Delta \mathbf{H} \Big)$$
(6.1)

$$\dot{\mathbf{H}}^{k} = -\boldsymbol{\mathcal{D}}^{k} \times \mathbf{E}^{k} + (\mathcal{M}^{k})^{-1} \mathcal{F}^{k} \Big( \Delta \mathbf{H} - \mathbf{\hat{n}} \cdot (\mathbf{\hat{n}} \cdot \Delta \mathbf{H}) - \mathbf{\hat{n}} \times \Delta \mathbf{E} \Big)$$
(6.2)

#### CHAPTER 6. HIGHPERMESHES PROJECT

The right hand side of both equations is divided into two parts, namely, the volume and the surface kernel. The first terms are the rotation of the magnetic field  $\mathcal{D}^k \times \mathbf{H}^k$  and the electric field  $-\mathcal{D}^k \times \mathbf{E}^k$ . These arithmetic operations are executed for all volume nodes on the tetrahedra. The following listing 6.1 shows a commented implementation of this kernel.

```
Listing 6.1: Volume kernel of DGTD Maxwell solver
```

```
// Volume kernel "for" loop over all mesh cells (for each mesh entity)
auto volumeKernelLoop = HPM::ForEachEntity(
AllCells,
std::tuple(
Read(Cell(fieldH)),
                         // electric field E
                        // magnetic field H
Read(Cell(fieldE)),
ReadWrite(Cell(rhsH)), // right hand side of H
ReadWrite(Cell(rhsE))), // right hand side of E
[&](const auto &element, const auto &, auto &lvs) {
// get Jacobian transformation matrix
 const Mat3D &D = element.GetGeometry().GetInverseJacobian()*2.0;
// derivatives of E and H fields in the current cell for all volume
    nodes (numVolNodes = 20 for third polynomial order)
 HPM::ForEach(DG::numVolNodes, [&](const std::size_t n) {
  Mat3D derivative_E, derivative_H;
// get current local values (lvs) of H and E fields for cell volume
   nodes
  const auto &fieldH = dof::GetDofs<dof::Name::Cell>(std::get<0>(lvs));
  const auto &fieldE = dof::GetDofs<dof::Name::Cell>(std::get<1>(lvs));
// compute derivatives of E and H fields for local volume nodes:
  HPM::ForEach(DG::numVolNodes, [&](const std::size_t m) {
      derivative_H += DyadicProduct(DG::derivative[n][m], fieldH[m]);
     derivative_E += DyadicProduct(DG::derivative[n][m], fieldE[m]);
  });
// get current local values (lvs) of right hand side (rhs) of H and E
   fields:
  auto &rhsH = dof::GetDofs<dof::Name::Cell>(std::get<2>(lvs));
  auto &rhsE = dof::GetDofs<dof::Name::Cell>(std::get<3>(lvs));
// compute rotations of E and H fields for all local nodes (n)
  rhsH[n] += -Curl(D, derivative_E);
  rhsE[n] += Curl(D, derivative_H);
 });
},
// openMP back end for parallel computation
HPM::internal::OpenMP_ForEachEntity<3>{});
```

The readability is a criterion of a modern clean code. This is taken into consideration in the HighPerMeshes project. Obviously, it is possible to understand the implementation here even without comments, as the variables and functions are given the same mathematical or physical names. Thus, allowing for a high productivity of the programmer. The second part of the numerical scheme are the second terms of the right hand side of the equations 6.1 and 6.2, namely, the flux term. Listing 6.2 shows the commented code of the surface kernel.

Listing 6.2: Surface kernel of DGTD Maxwell solver

```
// Surface kernel "for" loop over all mesh faces
auto surfaceKernelLoop = HPM::ForEachIncidence<2>(
 AllCells,
 std::tuple(
 Read(ContainingMeshElement(fieldH)), // H field of current element
 Read(ContainingMeshElement(fieldE)), // E field of current element
 Read(NeighboringMeshElementOrSelf(fieldH)), // H field of neighbor
 Read(NeighboringMeshElementOrSelf(fieldE)), // E field of neighbor
 ReadWrite(ContainingMeshElement(rhsH)), // right hand side of H
 ReadWrite(ContainingMeshElement(rhsE))), // right hand side of E
 [&](const auto &element, const auto &face, const auto &, auto &lvs) {
 // get faces local indices and calculate its normals coordinates
  const std::size_t face_index = face.GetTopology().GetLocalIndex();
  const RealType face_normal_scaling_factor = 2.0 / element.GetGeometry
     ().GetAbsJacobianDeterminant();
  const Vec3D &face_normal = face.GetGeometry().GetNormal() *
     face_normal_scaling_factor;
  const RealType Edg = face_normal.Norm() * 0.5;
  const Vec3D &face_unit_normal = face.GetGeometry().GetUnitNormal();
 // get mapping between element faces and neighbor ones
  const auto &localMap{DgNodeMap.Get(element, face)};
 // get current local values (lvs) of H and E fields for cell surface
    nodes (NumSurfaceNodes = 10 for third polynomial order)
 HPM::ForEach(DG::NumSurfaceNodes, [&](const std::size_t m) {
   const auto &fieldH = dof::GetDofs<dof::Name::Cell>(std::get<0>(lvs));
   const auto &fieldE = dof::GetDofs<dof::Name::Cell>(std::get<1>(lvs));
 // get neighbor H and E fields
   auto &NeighboringFieldH = dof::GetDofs<dof::Name::Cell>(std::get<2>(
      lvs));
   auto &NeighboringFieldE = dof::GetDofs<dof::Name::Cell>(std::get<3>(
      lvs));
 // compute differences of magnetic and electric fields dH and dE,
    respectively, on cells interfaces
   const Vec3D &dH = Edg * HPM::DG::Delta(fieldH, NeighboringFieldH, m,
```

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```
localMap);
 const Vec3D &dE = Edg * HPM::DG::DirectionalDelta(fieldE,
     NeighboringFieldE, face, m, localMap);
// compute the flux (flux_H, flux_E) for magnetic and electric fields
 const Vec3D &flux H = (dH - (dH * face unit normal) *
     face_unit_normal - CrossProduct(face_unit_normal, dE));
 const Vec3D &flux_E = (dE - (dE * face_unit_normal) *
     face_unit_normal + CrossProduct(face_unit_normal, dH));
// get current local values (lvs) of right hand side (rhs) of H and E
 auto &rhsH = dof::GetDofs<dof::Name::Cell>(std::get<4>(lvs));
 auto &rhsE = dof::GetDofs<dof::Name::Cell>(std::get<5>(lvs));
// Compute surface integration of the flux over all surface nodes
 HPM::ForEach(DG::numVolNodes, [&](const std::size_t n) {
  rhsH[n] += DG::LIFT[face_index][m][n] * flux_H;
  rhsE[n] += DG::LIFT[face_index][m][n] * flux_E;
 });
});
},
// openMP back end for parallel computation
HPM::internal::OpenMP_ForEachIncidence<3, 2>{});
```

The time integration with Low Storage Runge Kutta method as described in chapter 3 is implemented in the HighPerMeshes Framework in a simple way as Listing 6.3 shows.

Listing 6.3: Runge Kutta kernel of DGTD Maxwell solver

```
// Runge Kutta kernel loop over all mesh cells (for each mesh entity)
auto rungeKuttaLoop = HPM::ForEachEntity(
AllCells,
std::tuple(
ReadWrite(Cell(fieldH)), // electric field E
ReadWrite(Cell(fieldE)), // magnetic field H
ReadWrite(Cell(rhsH)), // right hand side of H
ReadWrite(Cell(rhsE)), // right hand side of E
ReadWrite(Cell(resH)),
                         // resiual of H
                          // resiual of E
ReadWrite(Cell(resE))),
  [&](const auto &, const auto &iter, auto &lvs) {
//Runge Kutta stage (get Runge Kutta coefficients)
  const auto &RKstage = RungeKuttaCoeff<RealType>::rk4[iter % 5];
// get current local values (lvs) of H and E fields for cell volume
    nodes
  auto &fieldH = dof::GetDofs<dof::Name::Cell>(std::get<0>(lvs));
  auto &fieldE = dof::GetDofs<dof::Name::Cell>(std::get<1>(lvs));
// get current local values (lvs) of right hand side (rhs) of H and E
```

```
fields:
  auto &rhsH = dof::GetDofs<dof::Name::Cell>(std::get<2>(lvs));
 auto &rhsE = dof::GetDofs<dof::Name::Cell>(std::get<3>(lvs));
// get current local values (lvs) of residual (res) of H and E fields:
 auto &resH = dof::GetDofs<dof::Name::Cell>(std::get<4>(lvs));
 auto &resE = dof::GetDofs<dof::Name::Cell>(std::get<5>(lvs));
// Time step integration for all cell volume nodes
  HPM::ForEach(DG::numVolNodes, [&](const std::size_t n) {
   resH[n] = RKstage[0] * resH[n] + timeStep * rhsH[n];
    resE[n] = RKstage[0] * resE[n] + timeStep * rhsE[n];
    fieldH[n] += RKstage[1] * resH[n];
    fieldE[n] += RKstage[1] * resE[n];
   rhsH[n] = 0.0;
    rhsE[n] = 0.0;
  });
},
// openMP back end for parallel computation
HPM::internal::OpenMP_ForEachEntity<3>{})
```

Writing the output from the parallel processes is possible using the writeLoop method. This allows writing the field results for each time step or at the end of the computation in the output files, which can be visualized or processed. As an example for this, a simulation with initial value problem in free space has been done. The computational domain here is a cube and the boundary condition is perfect electric conductor (PEC). Figure 6.1a visualizes the numerical solution of electric field component  $E_y$  resulted from DGTD Maxwell solver of HighPerMeshes for unstructured grid.



(a) partition dg nodes

(b) partition manipulated nodes

Figure 6.1: The component  $E_y$  of the electric field in a cubic cavity of (a) the numerical solution resulted from DGTD Maxwell solver for unstructured grid and (b) post processing manipulated solution for a structured one that have high resolution (51 × 51 × 51).

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Performing post processing manipulation for this result delivers a numerical solution for a structured grid that has a user defined resolution. This is displayed in figure 6.1b. The resolution here is  $(51 \times 51 \times 51)$ .

The same simulation is distributed on four processes in order to test the parallelization of HighPerMeshes. Figure 6.2 visualizes the manipulated  $E_y$  component for a structured grid. The results in figure 6.1 and 6.2 are validated quantitatively using another Maxwell solver.





(b) Partition 2



(c) Partition 3

(d) All 4 partitions gathered together

Figure 6.2: The result from different partitions of the component  $E_y$  of the electric field in a cubic cavity. (a), (b) and (c) display three partitions of the simulation domain from different processes, while (d) is the gathered results from all four processes.

#### 6.1 DGTD MAXWELL SOLVER IMPLEMENTATION IN HIGHPERMESHES

# 7

## Conclusion and outlook

In this work, optical opposition phenomena observed for light scattered from powder-like surfaces are studied and numerically analyzed. These are the negative polarization and intensity surge near backscattering. HPC resources are employed for solving this light scattering problem and implementing parallel code for this goal. The applied numerical model is based on the DGTD method and the used code is parallelized. As well, working on development of HighPerMeshes framework is progressing, which is also based on DGTD method and will be further developed. Simulations of light scattering from structures with different geometries are performed. These structures include single particles and layers of up to ten particles. Constituents shapes are cubes, faceted spheres and ellipsoids, and random irregular particles. The particles have sizes much larger than the wavelength of incident light.

The double scattering coherent mechanism is confirmed. Single particles with considered parameters do not produce negative polarization near backscattering. In contrast, all the considered structures with two and more particles can produce it. It, however, depends on the geometric conditions of the scatterers.

Total backscattering response from the considered structures is formed by single and double scattering. The polarization of these components is different. Total polarization is the sum of both. Whether the negative polarization feature appears in the scattering angle curve depends on the interplay between these components. Dominating single scattering results in enhanced intensity scattered backwards and suppressed negative polarization. So, that the total polarization becomes always positive. This is observed for structures with ellipsoids, cubes and irregular particles, where constituent form large surface areas perpendicular to the light incidence direction. For more random topographies that form optimal angles between surface elements the relative contribution of single scattering is reduced and double scattering becomes significant and negative polarization gets enhanced. Another reason reducing double scattering and, correspondingly, negative polarization is large distance between constituents. Thus, dense packing of particles is an enhancing factor of negative polarization which is in agreement with experimental measurements of compressed absorbing powder samples.

Numerical analysis of double scattering in two-particle structures with different shapes of constituents shows that the interference mechanism can result not only in negative polarization but also in no polarization or even strongly enhanced positive polarization. The negative polarization branch survives after averaging over many samples and distances between constituents.

Simulation results show that backscattering intensity can be enhanced in a broad range of scattering angles due to single scattering from constituents with favorable orientations. However, no direct correlation has been found between intensity surge and negative polarization at least for the considered structures.

As a future aspect, it is interesting to study the effect of surface roughness of random irregular particles of different scales regarding to the wavelength of incident light. As well, cluster of particles that have various sizes and different absorbing materials are also interesting for characterizing powder topologies and materials by analyzing the light scattered by them.

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## Notations

Acronym	Meaning
PDEs	Partial differential equations
GO	Geometrical Optics
FDTD	Finite difference time domain method
DDA	Discrete Dipole Approximation
T-matrix	Transition Matrix method
HPC	High performance computing
DGTD	Discontinuous Galerkin method in time domain
FEM	Finite element method
LSRK	Low storage Runge-Kutta method
PML	Perfectly matched layer
PEC	Perfect electric conductor
TF/SF	Total field / scattered field technique
CPUs	Central processing units
GPUs	Graphics processing units
FPGAs	Field programmable gate arrays
MPI	Message passing interface
GRF	Gaussian random field shapes

## Symbols

Symbol	Meaning
θ	Scattering angle
$\alpha$	Phase angle
$\mathbf{E}$	Electric field
Η	Magnetic field
D	Electric induction
В	Magnetic induction
Р	Polarization
J	Electric current density
ρ	Volume electric charge density
$I_{\parallel}$	Intensity measured in parallel plane to the incident one
$I_{\perp}$	Intensity measured in perpendicular plane to the incident one
m	Refractive index
r	Space vector
(x,y,z)	Cartesian coordinates
t	Time
$\varepsilon_0$	Permittivity in vacuum
$\varepsilon_r$	Relative permittivity
$\mu_0$	Permeability in vacuum
$\mu_r$	Relative permeability
ω	Angular frequency
k	Wave number
c	Speed of light
$\lambda$	Wavelength of incident light
Ι	Stokes vector
Ι	Intensity of light
Q	Axis dominance of polarization
U	Digonal dominance of polarization

Symbol	Meaning
V	Circular domonance of polarization
$\mathbf{S}$	Amplitude scattering (Jones) matrix
$oldsymbol{\psi}$	A form of amplitude scattering matrix
$\hat{lpha}$	Parallel unit vector to the scattering plane
$\hat{oldsymbol{eta}}$	Perpendicular unit vector to the scattering plane
$\mathbf{Q}$	Matrix of material constants
$\mathbf{F}$	flux
ξ	single six component vector of unknowns
$\kappa(\mathbf{r})$	Electrical conductivity
ε	Permittivity
$\mu$	Permeability
$\hat{\mathbf{e}}_{j}$	Cartesian unit vectors with $j \in \{x, y, z\}$
Ω	Simulation domain
K	Number of all cells of computational domain
$\mathcal{N}_{nodes}$	Total number of nodes for each cell
p	polynomial order
$\mathcal{L}_i$	Lagrange polynomials
$ ilde{oldsymbol{\xi}}_n^k$	Expansion coefficients
$\eta_n$	Local polynomial basis
$\mathcal{ ilde{R}}$	Residual
$\mathcal{D}^k$	Spatial differentiation matrix
$\mathcal{M}$	Mass matrix
${\cal F}$	Face matrix
Ζ	Impedance
Y	Conductance
$\hat{x}, \hat{y}, \hat{z}$	Auxiliary Cartesian coordinates
$A_n, B_n, C_n$	Runge-Kutta coefficients
R	Radius of the circumscribing sphere around the particle
kR	Size parameter