Development of future spray imaging techniques using General Purpose GPU accelerated Monte Carlo simulation

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Abstract

The past decade has seen the development and application of emerging laser techniques for spray imaging. Two noticeable examples are Ballistic Imaging (BI) and Structured Laser Illumination Planar Imaging (SLIPI). The main motivation in developing such novel techniques was to filter out the blurring effects introduced by multiple light scattering in order to obtain reliable two-dimensional qualitative and quantitative spray information. In parallel to this experimental development, Monte Carlo (MC) simulation of light propagation and scattering through spray systems has also been initiated. While the MC simulation is a powerful and versatile tool for modeling various spray geometries and detection schemes on a single computer, its main drawback remains its long computational time. However, since 2007 a programming approach, named Compute Unified Device Architecture (CUDA), has been created for performing general purpose calculations on Graphics Processing Unit (GPU), as a data-parallel computing device. Thanks to the continuously increased number of cores in combination with larger memory bandwidth, recent GPUs offer considerable extended resources for general purpose computing. In this article, we describe an accelerated version of a validated MC model (originally presented at ICLASS-2006), for the simulation of laser light propagation in sprays. The code is now capable of running the calculations on a modern GPU card, showing a ~100x increase in simulation speed compared to the original version of the code. Thanks to these new possibilities, the MC model presented in this article allows detailed performance analysis of various laser imaging techniques. This is demonstrated for BI where a time-gating approach is used and for SLIPI where a modulation-based filtering is employed in the spatial domain.

Introduction

Due to large improvements in cameras (higher sensitivity, larger dynamic range, faster recoding frame rate *etc*) and laser technology (higher pulse power, higher repetition rate, *etc*) the use of laser imaging techniques for spray characterization has become more and more attractive over the past two decades. The advantage of laser imaging techniques over point measurements remains in the possibility of rapidly obtaining two-dimensional spray information, as well as investigating in detail spray breakups from successive single-shot images. Nevertheless, it is well known that the major source of errors, while imaging a spray with visible light, originate from the large detection of multiple light scattering. To avoid such issues, some researchers have switched the incident wavelength to X-rays light (largely avoiding scattering effects and considering absorption instead) [1] while others have developed more advanced imaging techniques based on a variety of filtering strategies [2,3]. This intense activity in the development of new spray imaging techniques is mostly based on experimental testing. However, due to the complexity of the problem (polydispersity, inhomogeneity and transient nature of spray systems) one optical system can perform more or less efficiently from one spray to another. Most importantly it is of interest to quantify the filtering capability from different approaches and compare them in various situations. It has been reported that this optimization could be performed by modeling the light propagation through sprays using Monte Carlo (MC) simulation [4]. Even though the MC method is considered as "gold standard", due to its accuracy and flexibility in considering inhomogeneous three-dimensional geometries, its main limitation remains the large computing time required on a single computer. The main concept behind a MC algorithm is to break

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down a complex problem into a smaller and more easily defined set of calculations which are repeated a large number of times. Different calculation paths include the use of random numbers and a succession of probability density functions. This random sampling process must be sufficiently repeated in order to reduce statistical fluctuations. As the iterations are performed independently from each other, the overall simulation is highly parallelizable.

A graphics card which is able to execute non-graphical tasks is referred to as a General Purpose Graphics Processing Unit (GP-GPU). The benefit of using a GP-GPU is due to its capability to perform calculations on multiple input data simultaneously. On modern hardware, one single instruction has the potential to finish the calculation on hundreds of input parameters, while the Central Processing Unit (CPU) would finish the same calculations for the first few input parameters only. Thanks to these new capabilities, tasks which previously required significant computational time can now be executed several orders of magnitude faster. One task which benefits from this recent increase in speed is the Monte Carlo modeling.

This article focuses on the GP-GPU acceleration of a Monte Carlo code specially designed for the simulation of light propagation and scattering in spray systems. Details regarding the original development and validation of the code can be found in [5]. Thanks to its new capabilities of the code has been used in this article to study both, how a time-gated approach is capable of increasing image contrast (used in Ballistic Imaging [2]) and how the structured illumination approach (used in SLIPI [3]) is capable of rejecting the multiple light scattering intensity.

Modelling of the propagation of laser radiation in sprays

Definition of the spray region where the Monte Carlo simulation is applicable

The definition of "*dense spray*" diverges in between experimentalists, diagnosticians and modelers. In this article we provide a definition from an optical point of view where a spray can either be "*optically dense*" or "*optically dilute*". In an optically dense spray, photons interact in average, more than once with the immersed droplets. On the contrary, in a dilute spray photons interact less than once in average making the single scattering approximation valid in those conditions. Following this and respecting the definition from A. H. Lefebvre stating that "a spray is a system of droplets immersed in a gaseous continuous phase", the near-field spray region of an atomizing spray, which might contain an intact liquid core or a liquid sheet, cannot be defined as a dense spray, but can instead be described as the *"spray formation region"*. The far-field region of an atomizing spray becoming, then, the *"spray region"*. An illustration supporting this description is provided in Figure 1.

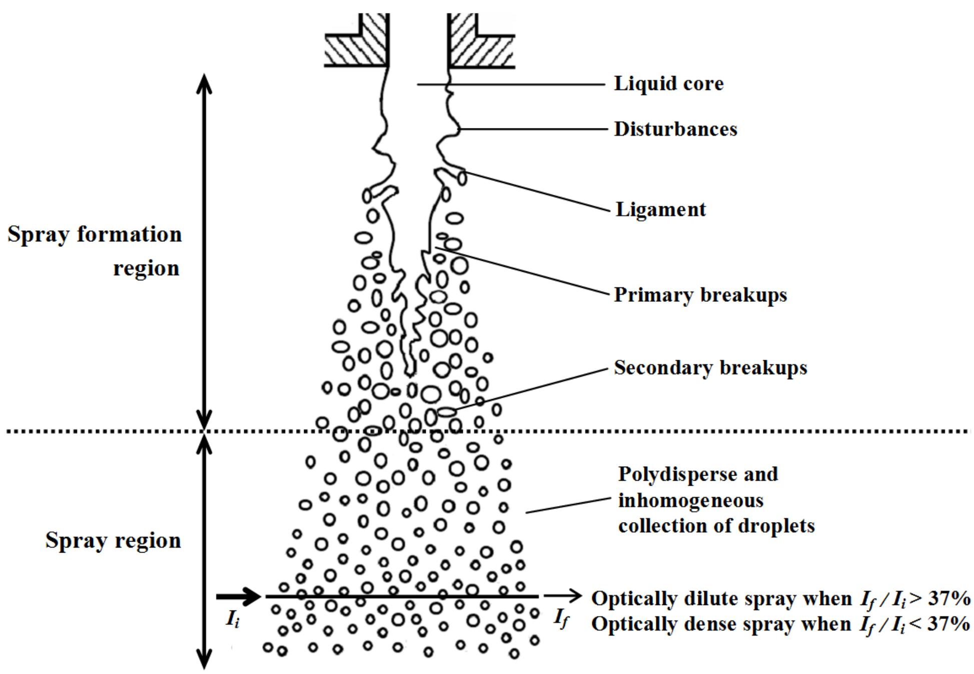


Figure 1 Illustration of the structure of an atomizing spray. The spray region can either be optically dilute or optically dense depending on the droplets number density, the droplets size and the illumination wavelength. As indicated in the figure a measure of light transmission I_f/I_i allows defining if the spray is optically dense or dilute for a given wavelength. The MC simulation presented here is only applicable in the spray region.

Light propagation in the spray region

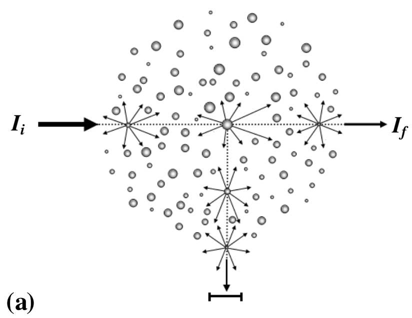
The propagation of a laser beam through a spray system is subject to attenuation and multiple scattering effects. These processes introduce errors in the measurement of droplet size and concentration as well as it blurs the recorded images, providing unfaithful qualitative description of the investigated spray. These processes are described as follows:

1- Laser extinction: Light beam attenuation along the incident direction due to both scattering and absorption. Depending on their position along the laser line-of-sight, droplets are not illuminated with the same light intensity (see Fig.2a).

2- Signal attenuation: Attenuation between the incident laser beam (or sheet) and the detector (also called out-of-plane attenuation). It corresponds to "secondary scattering" from droplets lying between the probe beam and the detector (see Fig.2a).

3- Multiple scattering: "Extraneous light" detected after being scattered by a number of the surrounding droplets (see Fig.2b).

The magnitude of error introduced by each of these processes varies with position, in a manner dependent on the spray geometry. Corrective solutions are unique for each source-detector configuration and for each spray structure. The most flexible way to understand and quantify the amount of error introduced by attenuation and multiple scattering in practical optical diagnostics of a spray is to simulate the problem.



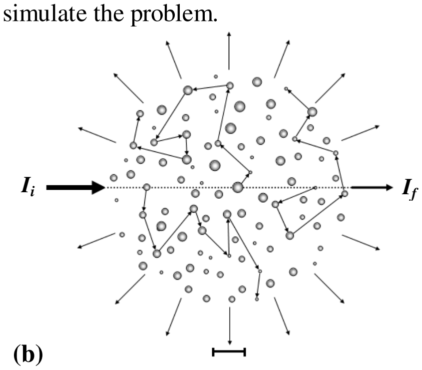


Figure 2 Illustration of light attenuation (a) and multiple scattering (b) when probing the spray region with a laser beam. The incident radiation is attenuated due to both scattering and absorption. Depending on the position along the laser beam, particles are not illuminated with the same energy. The singly scattered photons have a probability to be scattered more times while exiting the spray volume, as shown in (b).

The Radiative Transfer Equation

The radiative transfer theory is a theoretical model for the transport of photons through a scattering medium. The method ignores the behavior of the component wave amplitudes and phases, and treats photons as point particles. The theory is based on the central Radiative Transfer Equation (RTE) (or equation of radiative transfer). The RTE is a balance of energy between the incoming, outgoing, absorbed, scattered and emitted photons through a volume element. For the case of a laser beam propagating in a homogeneous spray volume (meaning that the number density of droplets N is constant), the RTE is given as:

$$\underbrace{\frac{1}{c}\frac{\partial I(\vec{r},\vec{s},t)}{\partial t}}_{(a)} = \underbrace{-\bar{\mu}_e I(\vec{r},\vec{s},t)}_{(b)} + \underbrace{\bar{\mu}_s \int_{4\pi} f(\vec{s}',\vec{s}) I(\vec{r},\vec{s},t) d\Omega'}_{(c)}$$

$$\text{with} \quad \bar{\mu}_e = \bar{\mu}_s + \bar{\mu}_a = N \cdot (\bar{\sigma}_a + \bar{\sigma}_s)$$

where t is time, $d\Omega'$ is the solid angle around $\vec{s}'$ and c is the speed of the light in the surrounding medium. The scattering phase function, $f(\vec{s},\vec{s}')$, describes the probability for a photon with an initial direction $\vec{s}$ to be scattered into the direction $\vec{s}'$ after a scattering event. The RTE can be summarized as follows: the change of radiance along a line of sight , term (a), corresponds to the loss of radiance due to the extinction of incident light, term (b), plus the amount of radiance that is scattered from all other directions $\vec{s}'$ into the incident direction $\vec{s}$ shown in term (c). The total extinction represented by term (b) equals the radiance lost due to scattering of the incident light in all other directions and the radiance that is absorbed at each light-droplet interaction (if the droplets are absorbing at a the excited incident wavelength). RTE is applicable for a wide range of turbid media including spray systems; however the analytical solutions are only available in rather simple circumstances where assumptions and simplifications are introduced to reduce the equation to a more tractable form [6,7].

Since there are no analytical solutions available to the transport equation in realistic cases, numerical techniques have been developed. The most versatile numerical solution to solve the RTE is based on the Monte Carlo approach.

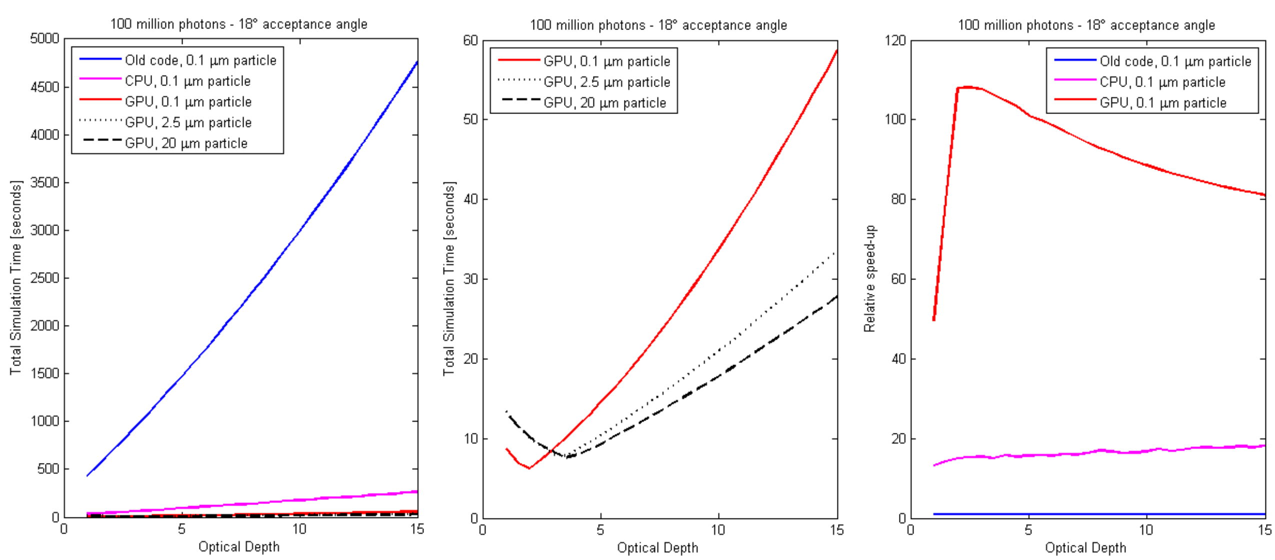
The Monte Carlo simulation

In 2006, a MC model has been developed and validated [4,5] for the investigation of light scattering in sprays. The main assumption of the MC technique is to define the source light as point entities representing photon packets. Each photon enters the simulated medium containing scattering and absorbing centers. These centers correspond, in the case of a formed spray, to spherical droplets. Photons are characterized with an initial direction and each photon is tracked as it travels through the spray medium. The photon trajectory is governed by probability density functions defined beforehand: the probability that a photon is scattered, the probability that it is absorbed and the probability to follow a new direction of propagation after a scattering event. An exhaustive description of the MC model would be too long to be provided in this article. However, the reader can have access to a complete description of the MC code used here and of its original algorithm in [4,5].

General Purposes computing on Graphics Processing Units: GP-GPU

The original purpose behind the development of GPU cards was to speed-up the rendering of three-dimensional vector graphics used in computer games. The rendering step consists of a large number of vector and matrix multiplications where the final two-dimensional images are made of textured and colored triangles. Even though the graphics card had good capabilities for performing vector and matrix operations, the results from the calculations could only be accessed as an image after the rendering had completed. Accessing image data in this manner was slow and as a result, past GPUs were not suited for general purpose calculations.

On a modern system multiple threads are executed in parallel. Threads running in parallel on a CPU are most often not limited in size or execution order. But due to the low amount of parallel threads, the overall speed can be improved on devices designed for parallel tasks. A typical CPU can run threads at speeds up to ~3 GHz. As it is often the case with parallel circuits, the clock speed of the graphics cards is lower than its "single threaded" cousins CPU. A typical modern GPU is running with a clock speed of ~1 GHz, which is three times slower than a CPU. However, due to the much larger amounts of parallel threads available to a GPU, parallel tasks allow it to reduce the total execution time compared to a CPU, by several orders of magnitude. This speed performance can be even more increased if two or three graphic cards are used in parallel, as shown by E. Alerstam *et. al* [8].



(a) **(b)** **(c)**

Figure 3 Execution time comparison for 100 million of photons launched, between the old MC code running on the CPU (Intel Core i7 950: only one core used), the new parallelized MC code running on the CPU (Intel Core i7 950: 8 cores used including hyper-threading) and the new code running on the GPU (Nvidia GeForce GTX 460, 2048 MB memory). In (a), the total time of the simulation as a function of the optical depth is shown for various sizes of non-absorbing water droplets suspended in air. (b) is a detailed representation of (a) for the GPU cases only. (c) is the relative speed-up of the new MC code in comparison with the old code. It is observed, in the case of 0.1 microns particles (near-isotropic scattering), that the code is able to speed-up the simulation by a factor of 100 times.

Due to the design limitations, multiple threads run on a GPU must perform the same type of operation during an equal amount of execution time. Threads on a GPU are divided into different workgroups. Each workgroup, by specification, must be independent of each other while threads inside a single workgroup are able to communicate with each other through shared memory and synchronization. In this article, a Monte Carlo model for light scattering in sprays has been optimized using GP-GPU. Final results showing the relative speed up between the old and the new code are shown in Fig.3(c) as a function of the optical depth [9].

Examples of simulations and results:

Description of the simulations:

The simulated medium consist of a cubic volume of dimension 10 mm x 10 mm x 10 mm, containing non-absorbing water droplets suspended in air. The refractive indices of the droplets and of the surrounding air are considered to be n_d= 1.33+0.0i and n_a= 1.00+0.0i respectively. The simulated scattering medium is considered monodispersed with droplets of either 2.5 μm or 20 μm in diameter. The incident wavelength is monochromatic and equals 532 nm. Two simulation configurations are investigated:

In the first configuration, the forward scattering light is detected and a 1ps time-gating approach is used together with a 100 fs and 1ps incident pulse respectively. A highly scattering spray is considered here, where the optical depth is fixed to OD = 10. An illustration of the simulation configuration is depicted in Fig.3(a). The aim of the simulation is to evaluate the ability of a 1ps time-gate in transmitting spatial information through a spray system. Imaging a square-wave test-chart provides a convenient method to estimate the spatial response of the time gated imaging system at a single spatial frequency. For the fundamental spatial frequency of the square-wave pattern, the contrast of the image, C, is defined as: $C = (I_{\max} - I_{\min})/(I_{\max} + I_{\min})$; where $I_{\min}$ and $I_{\max}$ are the respective minimum and maximum intensities of the imaged square-wave pattern. Two spatial frequencies equal to 1 lp/mm and 2 lp/mm are imaged and the corresponding contrast $C1$ and $C2$ have been calculated respectively. Similar type of simulation can be found in [10] where the performance of a a complete Ballistic Imaging system was investigated.

In the second configuration, the side scattering light is detected and a modulated laser sheet is used as the incident source of light. The optical density is in this case much lower and equals OD = 3. An illustration of the simulation configuration is depicted in Fig.4(b). The aim of the simulation is to evaluate the ability of Structured Laser Illumination Planar Imaging in filtering the light intensity from multiple scattering. A comparison with single scattering detection highlights the performance of the technique and its capability in providing accurate quantitative measurement of the extinction coefficient.

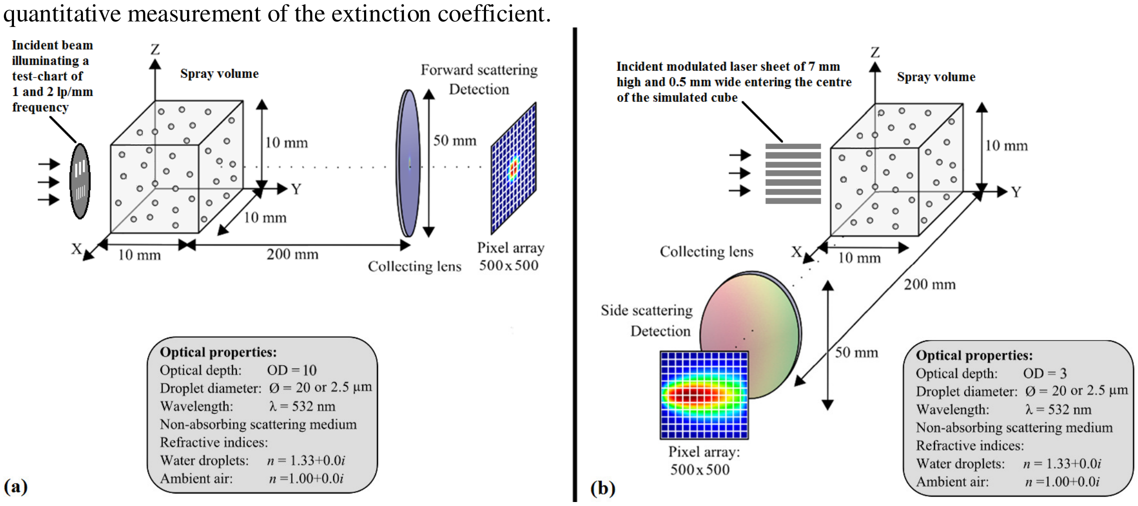


Figure 4 Description of the simulations: The outer dimensions of the medium are 10 mm x 10 mm x 10 mm. The 532 nm light source is positioned on the back face of the simulated volume and enters a spray system consisting of monodispersed water droplets. Droplets of 2.5 μm and 20 μm in diameter have been considered respectively. In (a) the collecting lens is detecting the forward light scattering and the medium is highly scattering with an optical depth of 10. In this simulation, a time gating approach is employed to investigate the image contrast enhancement. In (b) the collecting lens is detecting the light scattered at 90° and the medium has a moderate optical depth of 3. In this simulation, a structured illumination filtering approach is tested on a planar configuration (SLIPI). The capability in extracting the correct extinction coefficient is investigated.

Results for time-gated imaging: Application for Ballistic Imaging

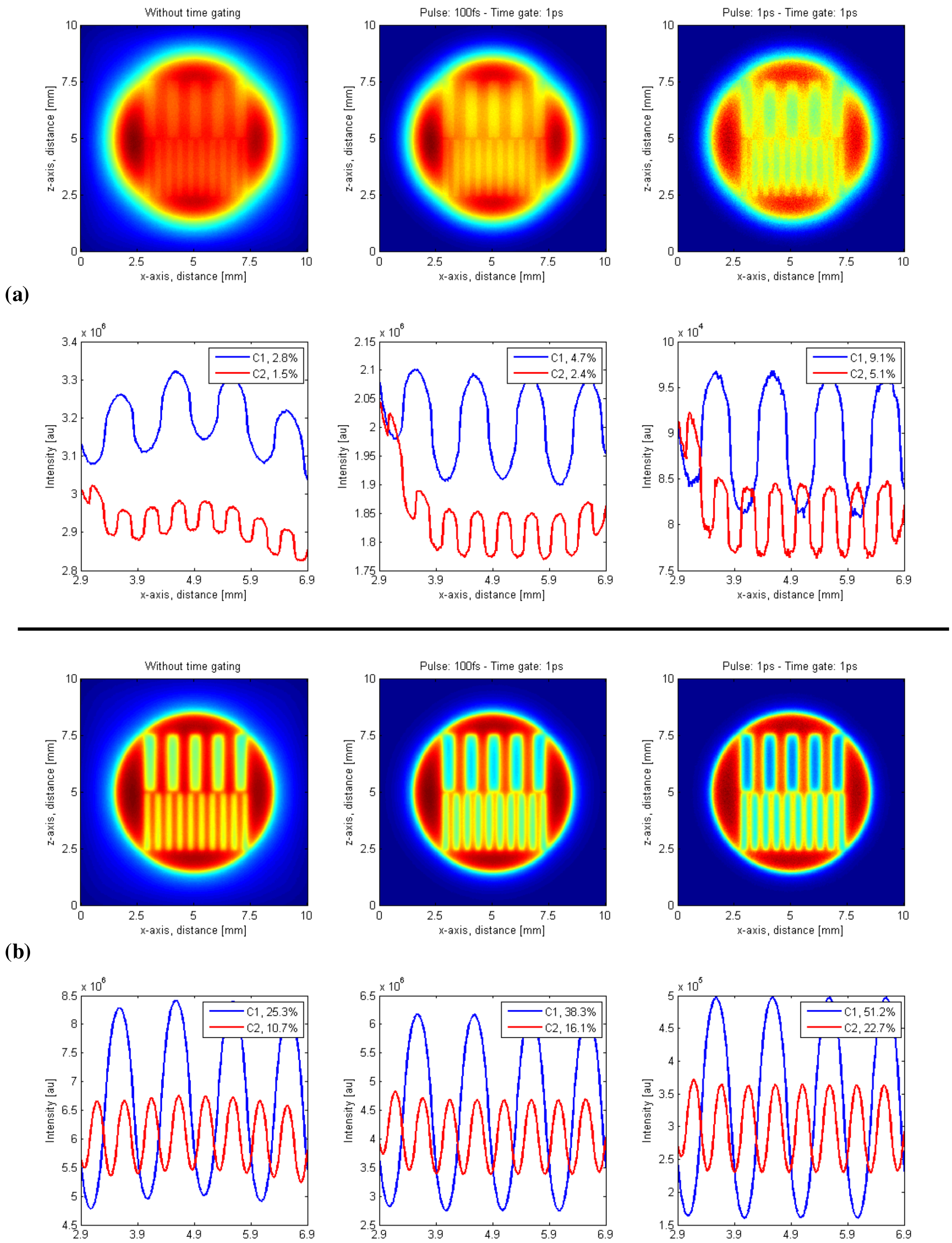


Figure 5 Image contrast comparison for three different cases. On the left no time-gating; in the centre, a 1ps time-gate is used with a 100 fs incident pulse; on the right, a 1ps time-gate is used with a 1 ps incident pulse. Water droplets of 2.5 μm and 20 μm are considered in (a) and (b) respectively. It is observed that the best contrast is obtained for the case of 1 ps time-gate with 1 ps imaging pulse. Also the 20 μm droplets exhibit a higher contrast due to the higher scattering lobe of the phase function around the 0° scattering angle.

Results for structured illumination filtering: Application for SLIPI

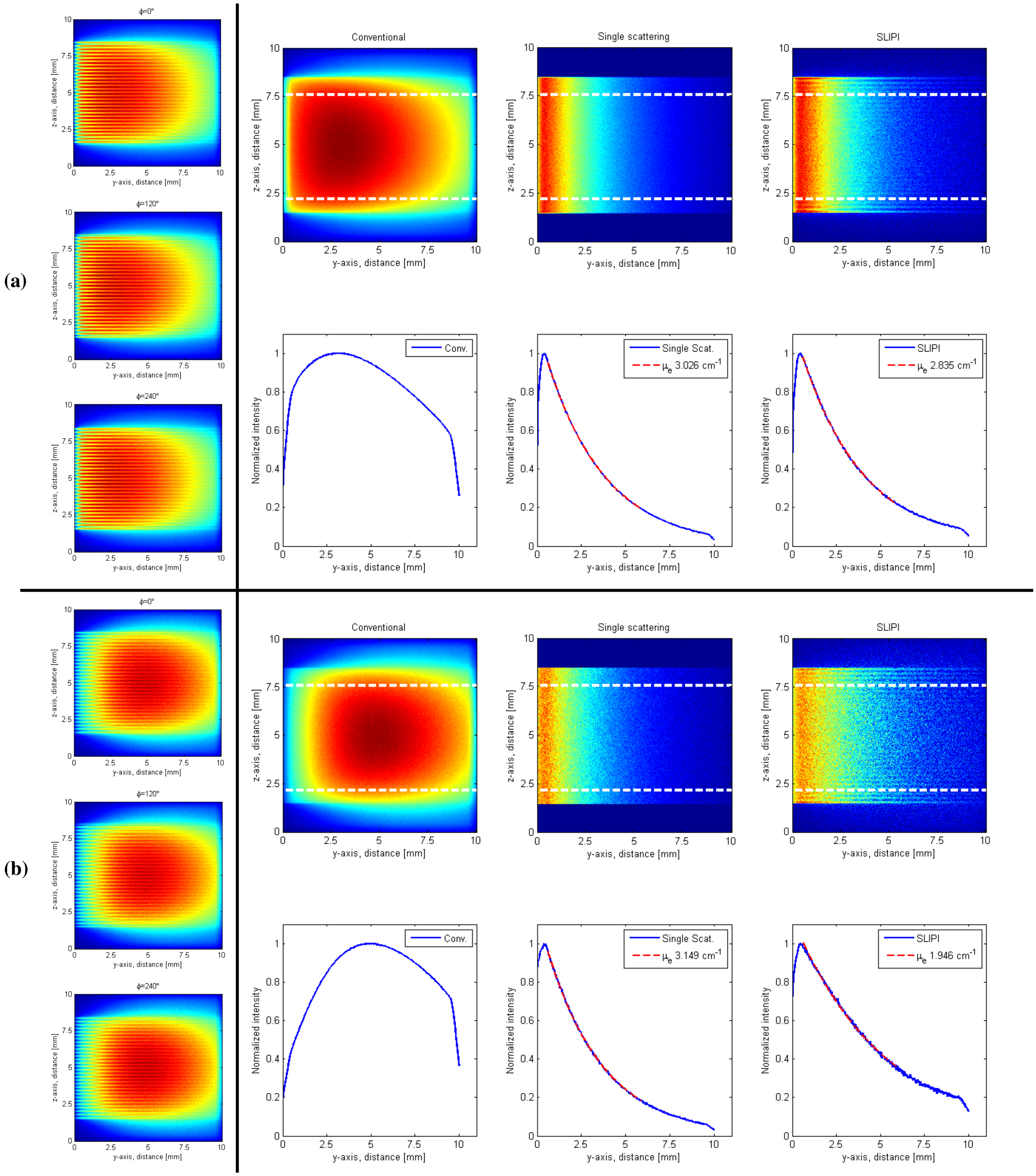


Figure 6 Results comparison between conventional planar imaging, single scattering detection and SLIPI. The vertically integrated signal is plotted below each image. The SLIPI image is reconstructed using three images where the incident laser sheet is modulated as shown on the left side of the figure. Water droplets of 2.5 μm and 20 μm are considered in (a) and (b) respectively. It is observed that an exponential decay, very close to the single light scattering detection (with an extinction coefficient ~3.0 cm^{-1}), can be extracted with SLIPI for the small droplets. For the large droplets discrepancies occurs with a measured extinction coefficient of ~2.0 cm^{-1}.

Discussion for the Ballistic Imaging results

It is seen from the results presented in Fig.5 that higher image contrast is obtained when the duration of the incident pulse matches with the time-gate applied. Experimentally, a ballistics imaging setup using a CS2 Kerr cell is capable of gating within 1-2 picoseconds. Using an incident pulse of 1 ps (instead of 100 fs usually used) helps in increasing the image contrast by a factor of 1.35 and 2 for the 2.5 μm and 20 μm droplets respectively. Further studies regarding contrast enhancement as a function of pulse duration and time-gate will be investigated in a near-future. A second observation is that even though the contrast is lower for the 2.5 μm, the square shape of the imaged test-chart remains well preserved. On the contrary, for the large droplets (20 μm), a more sinusoidal shape of the imaged test-chart can be observed, implying that image distortion and loss of information at high frequencies are induced by the scattering of light from the large droplets. A Fourier analysis of the resultant images could help in quantifying these distortion effects. Finally, in the case of the 2.5 μm droplets where light scatters at large angles from the forward direction, the effect of spatial filtering can be particularly efficient for contrast enhancement.

Discussion for the SLIPI results

It is seen from the results presented in Fig.6 that the exponential decay of the incident light intensity (represented by the single scattering detection) can be observed on the SLIPI images. By using an exponential fitting to the curves, a measure of the extinction coefficient is extracted. For the 2.5 μm and 20 μm droplets, an extinction coefficient of 2.8 cm^{-1} and 1.9 cm^{-1} are found respectively. As the extinction coefficient used in the simulation equals 3.0 cm^{-1}, this demonstrates that an accurate measure is observed for the small droplets while divergence occurs for the large ones. This is, once again, induced by the highly forward peak in the phase function of large particles, as demonstrated experimentally in [11]. By increasing the frequency of the modulated laser sheet could lead to more accurate results. Further simulations are required to better understand such filtering process.

Conclusions

The optimized code presented here allows solving complex scattering problems and simulating advanced imaging schemes, within a reasonable time-frame and without the need of expensive super computers. To give an order of magnitudes in term of computer performance, while the original code [6] presented at ICLASS-2006 was showing simulations using a number of 3 billion of photons, the results presented in this article are based on 600 billions of photons. This increase in number of photons sent through the simulated spray system allows better statistics, which is of particular importance at challenging detection conditions (small collection angle, ultra-fast time-gated detection, side scattering detection *etc*). Thanks to these new capabilities, advanced spray imaging techniques such as Ballistic Imaging and SLIPI can be analyzed in detail and further improved as exemplified in this article.

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