Simulation of light scattering and imaging of spray systems using the open-access software “Multi-Scattering”

Jönsson, Joakim; Berrocal, Edouard

Published in:
ILASS–Europe 2019, Proceedings of the 29th Conference on Liquid Atomization and Spray Systems, 2-4 September 2019, Paris, France

2019

Document Version:
Publisher's PDF, also known as Version of record

Link to publication

Citation for published version (APA):
Jönsson, J., & Berrocal, E. (2019). Simulation of light scattering and imaging of spray systems using the open-access software “Multi-Scattering”. In *ILASS–Europe 2019, Proceedings of the 29th Conference on Liquid Atomization and Spray Systems, 2-4 September 2019, Paris, France*

Total number of authors:
2

Simulation of light scattering and imaging of spray systems using the open-access software "Multi-Scattering"

Joakim Jönsson*, Edouard Berrocal
Division of Combustion Physics, Department of Physics, Lund University, Sweden
*Corresponding author: joakim.jonsson@forbrf.lth.se

Abstract

Spray systems contain a large amount of small droplets, which are responsible for multiple light scattering phenomena. When detected, photons that have been scattered multiple times blur the shape of liquid bodies present in the spray as well as the overall spray structure. This blurring causes issues with spray visualization and furthermore; multiple light scattering introduces large errors in quantitative measurements from image ratio techniques (e.g. LIF/Mie droplet sizing, two-color LIF thermometry, etc). The simulation of light propagation and scattering through spray systems is then necessary to understand the effects introduced by multiple scattering and to efficiently tackle the aforementioned issues. A reliable and predictive simulation tool allows for:
* Predicting the amount of multiple light scattering.
* Estimating the errors introduced by multiple scattering in quantitative spray measurements.
* Testing strategies for suppressing the intensity contribution from multiple scattering.
* Optimizing and assisting the development of different spray imaging techniques.
In this article we present an open-access software called "Multi-Scattering". It is a versatile online Monte Carlo simulation tool where photons are tracked through a cloud of spherical droplets. During the simulations process, each scattering event is described by the Lorenz-Mie theory. The numerical simulation is accelerated with the use of the parallel processing capabilities of modern computer graphics cards, known as general-purpose computing on graphics processing units, making those Monte Carlo simulations potentially in less than a minute. The simulations exemplified here demonstrate the use of Multi-Scattering for spray imaging application. This open access software is freely accessible to any researcher who would like to use it for their own spray application.
This is available at: `https://multi-scattering.com/`

Keywords

Optically dense sprays, Elastic scattering, Image contrast, Monte Carlo simulation

Introduction

Due to large improvements in cameras (higher sensitivity, larger dynamic range, faster recording frame rate etc) and laser technology (higher pulse power, higher repetition rate, etc) the use of laser imaging techniques for spray characterization has become increasingly attractive over the past three 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 main source of errors, while imaging an atomizing spray with visible light, originates from the detection of photons that have been scattered multiple times. This multiple scattering phenomenon is due to the presence of a large amount of small droplets. Their size and concentration will directly impact on the number of light-droplet interactions occurring in the spray. The more photons are being scattered, the more they will spread in different directions causing blur on the recorded image. This blur can affect the visualization of large liquid structures in the spray, as shown in Fig.1 and prevent the measurement of droplet parameters (e.g. size distribution, concentration, velocity and temperature). To suppress the unwanted effects caused by multiple light scattering, some researchers have developed a variety of optical filtering strategies such as time-gating [1], spatial Fourier filtering, Structured Illumination [2] and more recently two-photon fluorescence [3]. Other researchers have instead reduced the emission of the scattered radiation by switching the use of visible light to X-ray illuminations [4] where in this case, absorption is the dominant process. This active development of imaging techniques for spray characterization has been so far mostly based on experimental testing. However, due to the complexity of the problem related to polydispersity, inhomogeneity and the transient nature of atomizing sprays, optical filtering strategies might not perform as efficiently from one spray to another. In addition, it is important to be aware of the limits at which a given technique will or will not perform well. Such questions can be answered by accurately simulating the problem of light propagation through spray systems. A validated model provides the possibility of:

- Understanding the effects and quantifying the amount of multiple light scattering depending on the spray characteristics and the source/detector configuration.
- Predicting and assessing the capability of a technique in suppressing those effects.

It has been reported in the literature [5, 6, 7] that the most versatile and flexible way of modeling photon transport through scattering media, such as sprays, is by means of the Monte Carlo (MC) method. The main concept behind a MC algorithm is to break down a complex problem into a series of smaller sets of probability calculations which are repeated a large number of times. The different existing possibilities/paths are then sampled by using random numbers and a succession of probability density functions. This random sampling process must be sufficiently repeated a large number of times in order to reduce statistical fluctuations and obtain converging results. For the case of the simulation of light propagation through spray systems, several billions of photons need to be launched to reach satisfying statistics. Such requirement has been the main limit for using Monte Carlo simulation, especially when a collecting lens is used and only a portion of the total simulated light is contributing to image formation. However, as each iteration describing photon path in the spray is performed independently one from another, the overall simulation is highly parallelizable. Thus, Monte Carlo simulations can be executed on graphic cards [8, 9], a method known as a General Purpose Graphics Processing Unit (GP-GPU). We present here a novel online GP-GPU Monte Carlo software called “Multi-Scattering”, shown in Fig.2, specially designed for simulating light propagation and imaging through spray systems. As the software is freely accessible online, it can be used to any user interested in understanding effects related to multiple light scattering in spray imaging.

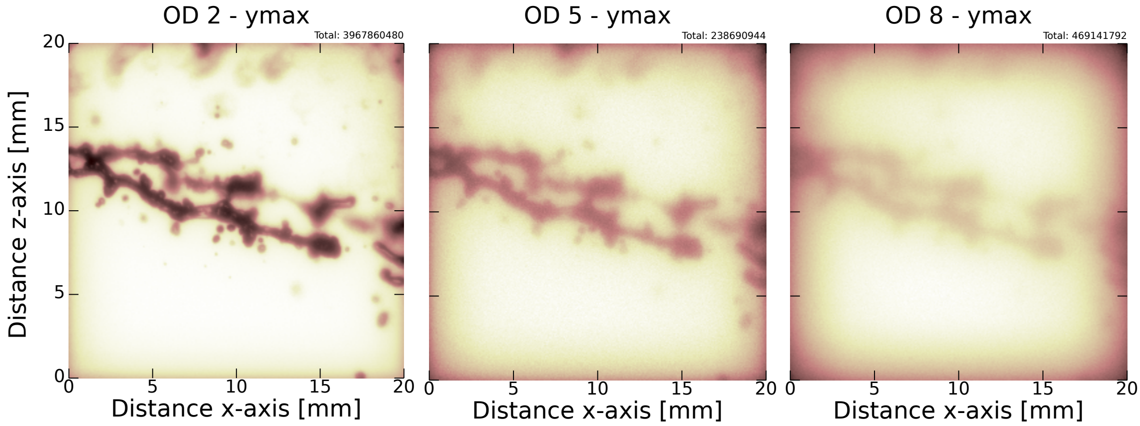


Figure 1. Example of simulation for spray shadowgraphy. The large liquid structures are blurred by the presence of 10 μm water droplets located in front of them. When the concentration of the droplets increases, corresponding to higher optical depth OD, blurring increases. At OD=2, only little blur occurs while at OD=8 where the liquid structures are not visible anymore.

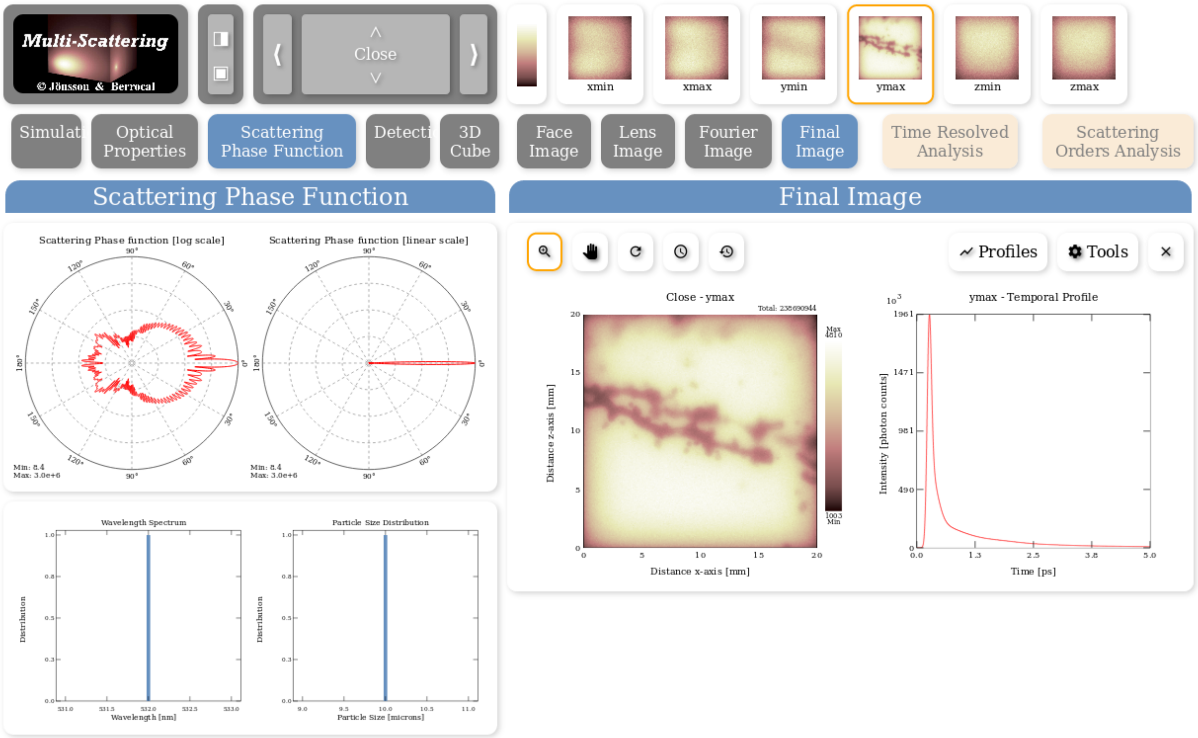


Figure 2. Screen-shot of the Multi-Scattering software where the output results of the simulations are shown together with the optical characteristics of the simulation. The scattering phase function generated from the Lorenz-Mie theory is shown here for the case of 10 μm water droplets illuminated at 532 nm.

In the first section of this article a general description of the simulation and of the algorithm architecture is provided. In section two, the acceleration of the code using GP-GPU is explained and a comparison between single to multi-threaded simulations is given. Finally, in section three, examples of simulations showing shadowgraphy images of liquid structures hidden behind clouds droplets are shown. Droplets size of 5 μm and 25 μm are respectively considered, and the results are compared.

General description of the simulation

In the field of laser diagnostics, the migration of photons through scattering media is generally described by the Radiative Transfer Equation (RTE) [10]. The RTE is a balance of energy between the incident, outgoing, absorbing and scattering radiation propagated through the medium. Since there are no analytical solutions available to the transport equation in realistic cases, numerical techniques have been developed and utilized. The most versatile and widely used numerical solution is based on the statistical Monte Carlo (MC) method, which is the approach used in Multi-Scattering. As shown in Fig.3 the Multi-Scattering simulation code is divided into two sections:
1) The Monte Carlo code that tracks photon packets in the scattering medium
2) The detection code that selects and collects the desired light exiting the scattering medium and form an image matrix.
At the beginning of the simulation, each photon packet is given an initial random position which is defined from a light source matrix. Since the matrix is a picture any incident beam profile can be used as input light source. In addition to the initial position, photon packets are assigned with an incident direction of propagation. Using those parameters, they are launched into the scattering medium and the distance l_{fp} along which they can travel prior to an interaction with a droplet is calculated using a random number ξ generated between 0 and 1, such as:

$$I(x) = -ln(\xi)/(\mu_s + \mu_a) \tag{1}$$

where μ_s and μ_a are the scattering and absorption coefficients, respectively. Once a light droplet interaction occurs, the amount of scattered light must be adjusted depending on the absorption properties of the droplet in respect with the incident wavelength. The albedo a is the fraction of photons being absorbed over the total extinction:

$$a = \mu_s/(\mu_s + \mu_a) = \mu_s/\mu_e \tag{2}$$

Photon packets start their journey with an initial weight $W_0 = 1$. At each interaction n the weight is reduced if the droplets are absorbing. The fraction of light being absorbed corresponds to:

$$\Delta W_a = W_n \cdot [\mu_a/(\mu_s + \mu_a)] = W_n \cdot (1 - a) \tag{3}$$

Finally the new photon weight is given as:

$$W_{n+1} = W_n - \Delta W_a \tag{4}$$

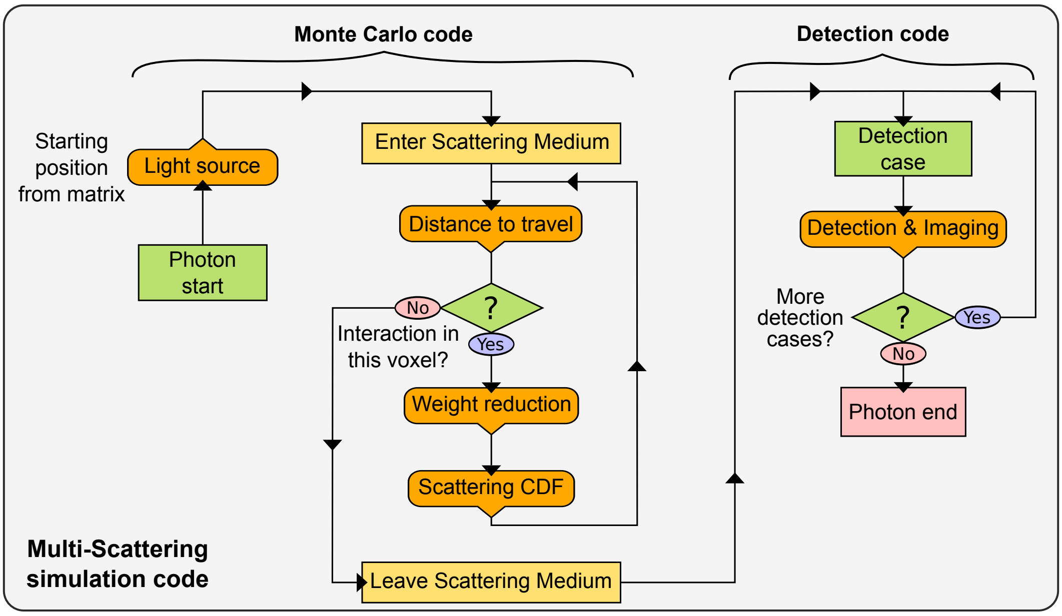


Figure 3. Flow chart of the Multi-Scattering simulation code. The loops start from the left where photons are assigned a starting position on the face of the scattering medium using a light source matrix. Once a photon packet enters the scattering medium a distance of light/droplet interaction is calculated. If the interaction is within the boundaries of the simulated volume, then it continues inside the scattering medium; otherwise it leaves, and the simulation continues to the Detection code seen to the right. Each available detection scheme processes the photon data and generates a number of resulting images.

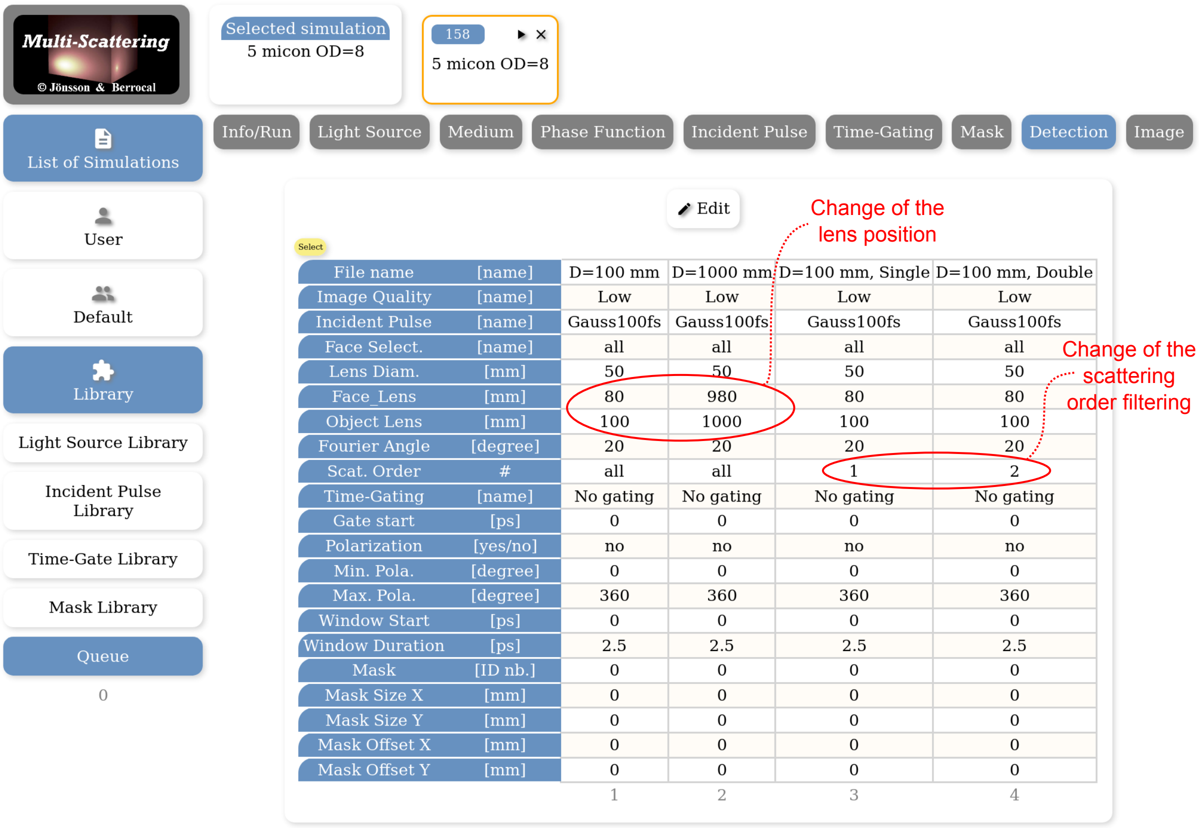
After a scattering event, a new photon direction, specified by the azimuth angle Θ and polar angle Φ, is calculated. This new direction is chosen by using the Cumulative Distribution Function (CDF) of the scattering phase function

and generating a random number. As the droplets are considered spherical, the CDF is pre-calculated from the Lorenz-Mie [11, 12] scattering phase function $f(\theta_s)$ which is dependent on the optical properties of:
- The surrounding medium (e.g. refractive index)
- The droplets (e.g. refractive index, droplets diameter)
- The incident light source (e.g. wavelength, polarization)

The scattering angle θ_s is generated from the CDF of $f(\theta_s)$ and using a random number $\xi \in [0, 1]$. As droplets are assumed to be perfectly spherical, their scattering phase function is symmetrical around the incident illumination direction. This makes the second scattering angle ϕ_s uniformly distributed in the range: $[0, 2\pi]$.
When a new propagation direction is defined, the position of the next scattering point is re-calculated, and the process repeated until the photon is either absorbed or exits the medium. The final propagation direction, position, number of scattering events, and the total path length are calculated at the end of each photon's journey within the scattering medium.

The second part of the simulation shown on the right side of Fig 3 is called the “Detection code”. Once photons exit the scattering medium, a number of detection conditions are set and only photons that meet those conditions are selected. A given detection case is defined by a number of parameters. For imaging, the most important parameters are the position and size of the collecting lens where photons reaching the lens will be the only ones contributing to image formation. Additionally, a number of filtering options can be further applied for a given detection case. For example, photons can be selected depending on the number scattering events, and they can be temporally filtered by using a given time-gate and/or spatially filtered by applying an aperture at the Fourier plane of the lens (spatial Fourier filtering). It should also be pointed out that the shape and duration of the incident pulse are included as a parameter.
Since a detection case is processed using its own parameters, it can be considered as a separate simulation from the Monte Carlo simulation code. This offers the possibility to set, not only one, but a number of detection cases where the same output data from the Monte Carlo code is being processed several times with different parameters by the Detection code, Fig.4.

The total number of photons that needs to be launched depends on the desired accuracy and on the detection characteristics. In order to reach acceptable statistics, a large number of photons must be launched. In fact, the exact solution of the Radiative Transfer Equation would be obtained for an infinite number of photons.



Change of the lens position

Change of the scattering order filtering

File name	[name]	D=100 mm	D=1000 mm	D=100 mm, Single	D=100 mm, Double
Image Quality	[name]	Low	Low	Low	Low
Incident Pulse	[name]	Gauss100fs	Gauss100fs	Gauss100fs	Gauss100fs
Face Select.	[name]	all	all	all	all
Lens Diam.	[mm]	50	50	50	50
Face_Lens	[mm]	80	980	80	80
Object Lens	[mm]	100	1000	100	100
Fourier Angle	[degree]	20	20	20	20
Scat. Order	#	all	all	1	2
Time-Gating	[name]	No gating	No gating	No gating	No gating
Gate start	[ps]	0	0	0	0
Polarization	[yes/no]	no	no	no	no
Min. Pola.	[degree]	0	0	0	0
Max. Pola.	[degree]	360	360	360	360
Window Start	[ps]	0	0	0	0
Window Duration	[ps]	2.5	2.5	2.5	2.5
Mask	[ID nb.]	0	0	0	0
Mask Size X	[mm]	0	0	0	0
Mask Size Y	[mm]	0	0	0	0
Mask Offset X	[mm]	0	0	0	0
Mask Offset Y	[mm]	0	0	0	0
		1	2	3	4

Figure 4. Screen-shot of the detection parameters set in the simulation. In this example, four detection cases are considered. In the first two, the collecting lens is located at different positions while in the last two cases, photons are selected depending on the number of scattering events they have been experiencing (defined as scattering order). Note that the software is not limited to four cases only and can include as many detection cases as desired. Also, the detection codes include a variety of filtering strategies such as time-gating, polarization and spatial Fourier filtering.

Acceleration of the code using GP-GPU

To achieve a high number of photons per simulation the Monte Carlo code needs to be as efficient as possible. As can be seen in Fig.3 each photon packets can be tracked individually and independently of other photon packets; therefore, it is possible split the simulation time by running the application on multiple threads. Commonly there are two ways to operate calculations on a computer in parallel. One way is to run the application on the central processing unit (CPU) and the other one is by using a graphics processing unit (GPU). Originally the GPU, as the name implies, was intended just for computing graphics but in recent years its capabilities have grown allowing it to perform general purpose (GP-GPU) calculations as well. There are some significant differences in how CPU and GPU operate.

This means that a given problem that can be quickly calculated using the CPU could be very slow when using the GPU and vice versa. CPU threads are primarily designed to work well with computational loads of arbitrary computational length. This feature is what limits the number of threads available on a CPU. The GPU on the other hand is designed with threads grouped together. Big chunks of memory are acceded by a thread group, and then the threads perform the same types of operations on all the data at once. When threads need to follow different calculation paths, some of the threads in the group have to be stalled while the other threads complete their tasks. When GPU threads can run unhindered, they vastly outperform the threads available on the CPU because there are many more threads available in each thread group of the GPU.

When a Monte Carlo method relies on the use of big chunks of memory in its calculation model it has the potential to benefit from the use of a GPU. The Multi-Scattering code relies on the use of Cumulative Distribution Functions and the final results are a collection of images. Thus, matrices are used both as input and output data. However, since photons are tracked through a random amount of scattering events the computer require different amounts of processing time to complete each iteration of the Monte Carlo loop. Most simulation cases require a large amount of photon packets for the final results to converge with satisfying statistics. Thus, large computational power is required for obtaining realistic results which was an important drawbacks of Monte Carlo simulation for photon transport through scattering media. With the current use of GP-GPU for Monte Carlo simulations, it is possible to gain simulation speed by over two orders of magnitude as originally shown in [8].

Satisfying the criteria of independent photon packets per thread and using matrices in the memory data structure; the first development of Multi-Scattering was directed from a single threaded nature to taking full advantage of the computer hardware available. With the updated code the simulations are now capable of running both faster and independently from the CPU. A benefit of the new source code is that it allows for one simulation to be spread on multiple graphics cards adding to the final speed boost. As a result, a single simulation runs now on 4 GPUs which are located in a single computer. A server made of three such computers has been built to run the simulations using Muti-Scattering.

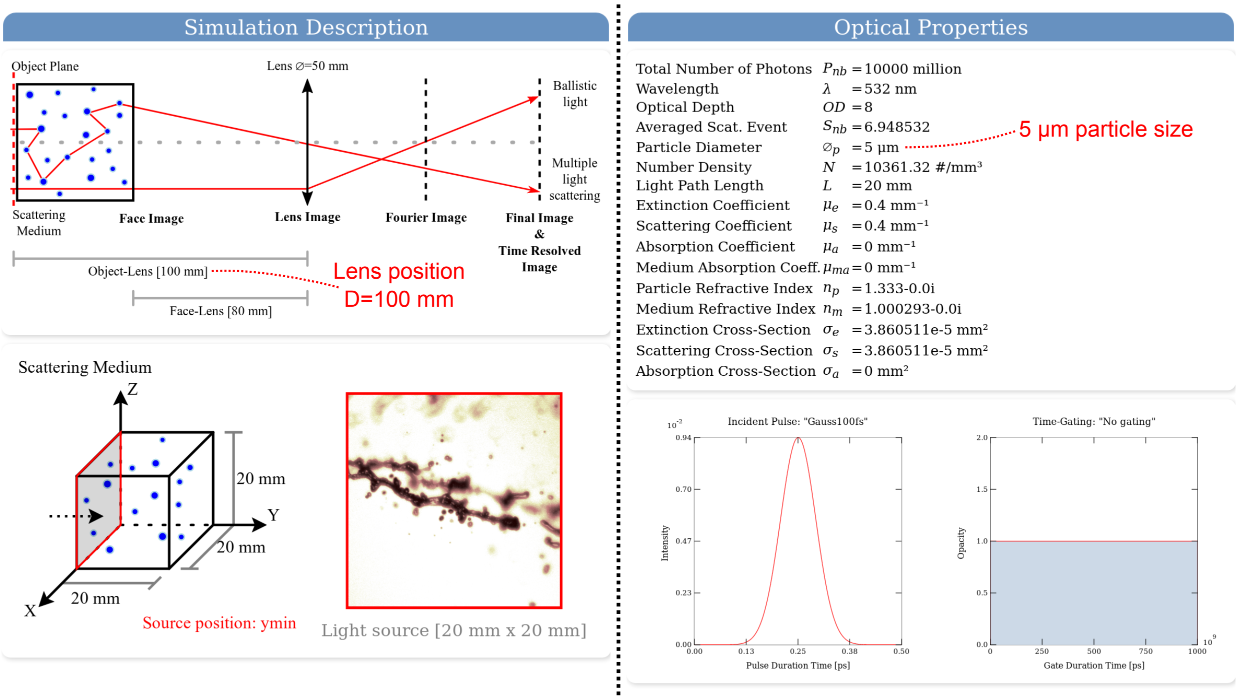
A speed comparison of our code can be seen in Table 1. By running the code on a single CPU thread and then comparing the time of execution to that when running it on a single GPU, a speed increase superior than 200 times is reached. With 4 GPUs connected to a single motherboard (a single computer) the increase in speed is now over 800 times, which now allows running spray simulation within less than a minute instead of half a day.

			Execution time (seconds)		
Case	**Hardware**		OD=2	OD=5	OD=10
A	Nvidia GeForce GTX 1080 Ti	4 units	2,7	3,1	4,8
B	AMD Ryzen Threadripper 2950X	16 threads	112,7	180,5	299,6
C	AMD Ryzen Threadripper 2950X	32 threads	80,7	124,9	204,4
D	Nvidia GeForce GTX 1080 Ti	1 unit	9,5	11,5	17,9
E	AMD Ryzen Threadripper 2950X	1 thread	1466,1	2515,5	4251,7
			Speed-up		
	Comparision	C & D	8	11	11
		E & D	154	219	237

Table 1. Speed comparison when launching 1 billion photons in the simulations. The CPU have 16 cores with the capacity of 32 threads in total. 16 threads can run independently, one for each core, while more threads have to share the resources. The most fair comparison is between test case C & D. C uses a single GPU and D is using all threads of the CPU. Going from a single CPU thread to GPU or multiple CPU threads can make significant differences.

Example of simulation

The basic idea behind this example is to show what will happen when the global structures of the spray are hidden by a cloud of droplets thus blurring the final results. This is achieved by using an experimental shadowgraphy image as input light source and using a simulated scattering medium to blur the transmission. In this example two simulations have been created. The first simulation is using 5 μm water droplets in air and the second simulation is using 25 μm water droplets in air. Apart from the particle size both simulations use the same input properties. The light source array that is used can be seen in Fig.5 as well as the dimension of the scattering medium and the positioning of the collecting lens in relation to the object plane. The position of the incident light source is indicated by the dotted arrow in the figure in the left side of the scattering medium. Each simulation has two basic detection cases seen in Fig.4. The first case has the lens positioned 100 mm from the object plane while the other has the lens positioned at 1000 mm from the object plane. The wavelength of the light source is λ=532 nm and the optical death is OD=5.



Total Number of Photons	P_{nb}	=10000 million
Wavelength	λ	=532 nm
Optical Depth	OD	=8
Averaged Scat. Event	S_{nb}	=6.948532
Particle Diameter	$\varnothing_p$	=5 µm
Number Density	N	=10361.32 #/mm³
Light Path Length	L	=20 mm
Extinction Coefficient	μ_e	=0.4 mm⁻¹
Scattering Coefficient	μ_s	=0.4 mm⁻¹
Absorption Coefficient	μ_a	=0 mm⁻¹
Medium Absorption Coeff.	μ_{ma}	=0 mm⁻¹
Particle Refractive Index	n_p	=1.333-0.0i
Medium Refractive Index	n_m	=1.000293-0.0i
Extinction Cross-Section	σ_e	=3.860511e-5 mm²
Scattering Cross-Section	σ_s	=3.860511e-5 mm²
Absorption Cross-Section	σ_a	=0 mm²

Figure 5. Screen-shot from the output website interface showing the description of the simulation and providing the optical properties.

The final results shown in Fig.6 are the results from transmission imaging. As the location of the lens is moved further away effects from image blur are reduced. For the 5 μm particle size the improvement is strongly visible while for the 25 μm only little improvement is observable. As can be seen in the graphs next to the imaging results, what happens when the lens is moved away is that the amount of late arriving photons is significantly reduced. The longer a photon remains in a scattering medium the more times it has been scattered. By limiting the number of late arriving photons images with higher contrast can be produced.

In Fig.7 the imaging results from the Fourier plane are shown. For the 5 μm particle size single scattering have a clear ring pattern while for photons that have scattered twice almost all the information of the scattering phase function have been lost. This means that the more the photons scatter the more they will spread out gaining wider angles. When the lens is moved from 100 mm to 1000 mm the effective collecting angle is reduced thus allowing only the ballistic and forward light scattering, reducing to some extent the contribution from multiple light scattering. For the 25 μm particle size in Fig.7 the ring pattern is still clearly visible even at after the photons have scatted twice. Thus, it follows that the photons will spread much less than compared to 5 μm particle size. Since photons to some extent preserve their initial direction even after scattering a few times it follows that it is much harder to reduce blurriness by moving the collecting lens.

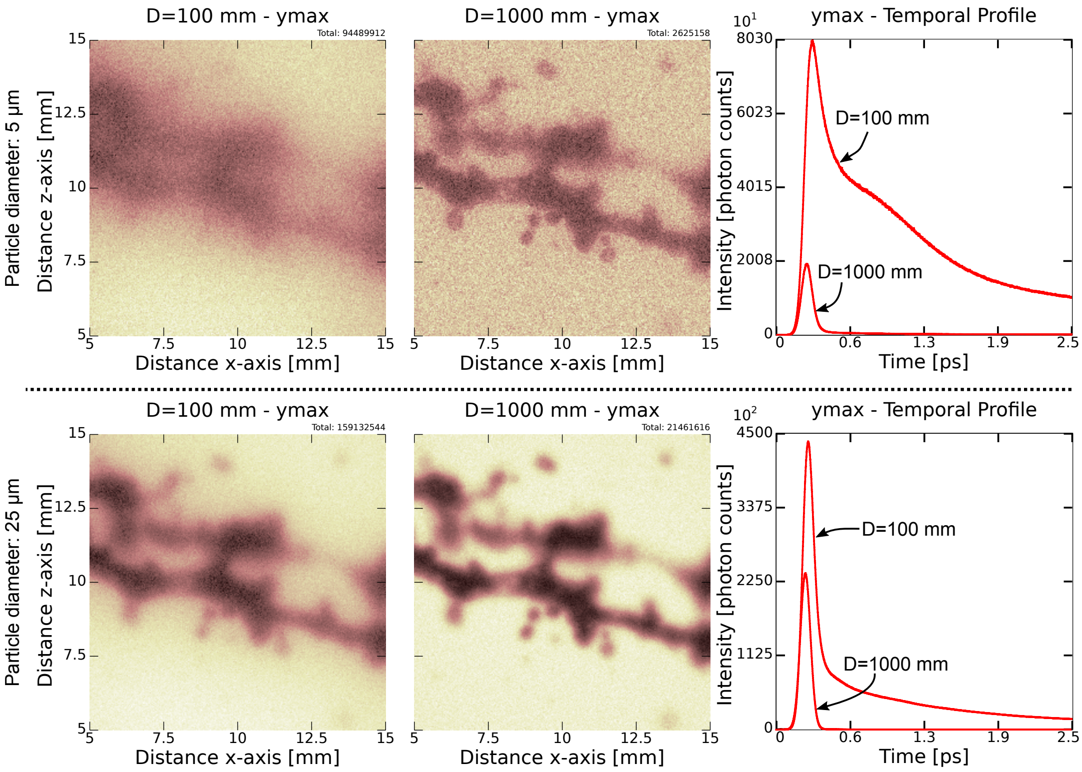


Figure 6. 5 μm respectively 25 μm water droplets in air. The first column has the collecting lens positioned 100 mm from the object plane while the second column has the lens positioned at 1000 mm from the object plane. All results are recorded with the optical depth OD=8.

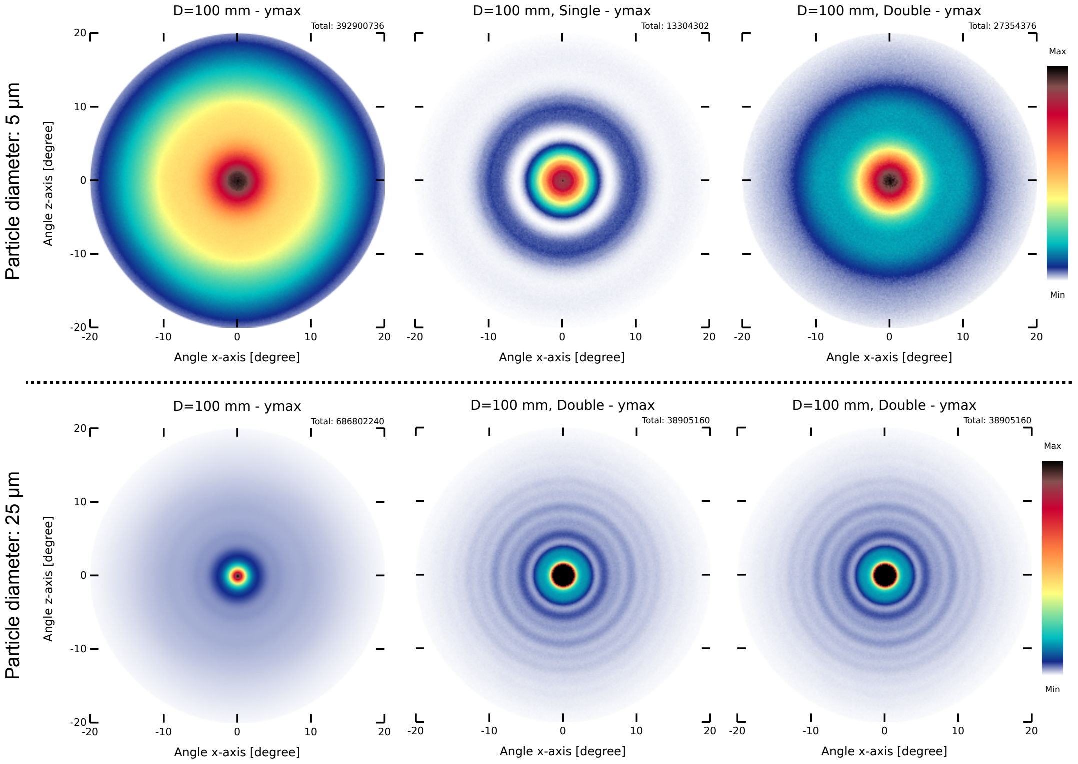


Figure 7. Resulting Fourier images from the Fourier plane of 5 μm respectively 25 μm water droplets in air. The position of the collecting lens is constant at D=100 mm while the particle size varies between the top and the bottom row. The *first* image in each row includes all photons. The *second* image only considers photons that have scattered exactly once and the *third* image only considers photons that have scattered exactly twice. The last two images for 25 μm have their maximum saturated to highlight the ring pattern.

Conclusions

A Monte Carlo simulation is a versatile tool able to simulate a turbid scattering medium consisting of a cloud of droplets. With an extensive user interface, simulations can be created easily and correctly without the need for prior deeper knowledge of the input variables needed. By the use of different light source matrices, added as normal images, numerous possibilities become available to both students and scientists who wish to understand and visualize the effects of multiple scattered light. It also allows researchers to gain a deeper and quantitative knowledge of their spray projects. With different numerical filters and the collection of useful statistical data results can be accurately analyzed. By having improved the simulation speed using modern computer graphics cards, GPUs, simulations can be launched and completed in a matter of minutes. By having shared simulation computers connected to;
`https://multi-scattering.com/`
the users do not need to by any expensive hardware. They do not need any programming skills and they do not need to buy any program licenses as the user interface already allows for quickly analyzing the results.

References

[1] Linne, M., Paciaroni, M., Berrocal, E. and Sedarsky, D., Proc. Combust. Inst. 32(2): 2147–2161 (2009).
[2] Berrocal, E., Kristensson, E., Richter, M., Linne, M. and Aldén, M., Opt. Express 16: 17870-17881 (2008).
[3] Edouard Berrocal, Chris Conrad, Jeremias Püls, Cord L. Arnold, Michael Wensing, Mark Linne, and Miguel Miranda, "Two-photon fluorescence laser sheet imaging for high contrast visualization of atomizing sprays," OSA Continuum 2, 983-993 (2019)
[4] Kastengren, A., Powell, C., Proc. Inst. Mech. Eng. D J. Automobile Eng. 221 (D6): 653–662 (2007).
[5] L. Wang, S. Jacques, and L. Zheng, “MCML - Monte Carlo modeling of light transport in multi-layered tissues,” Comput. Meth. Prog. Biol. 47, 131–146 (1995).
[6] Franck Jaillon and Hervé Saint-Jalmes, "Description and time reduction of a Monte Carlo code to simulate propagation of polarized light through scattering media," Appl. Opt. 42, 3290-3296 (2003)
[7] Jessica C. Ramella-Roman, Scott A. Prahl, and Steve L. Jacques, "Three Monte Carlo programs of polarized light transport into scattering media: part I," Opt. Express 13, 4420-4438 (2005)
[8] Alerstam, E., Chun Yip Lo, W., Han, T., Rose, J., Andersson-Engels, S. and Lilge, L., Biomed. Opt. Express 1: 658-675 (2010).
[9] Jönsson, J., Acceleration and optimisation of a Monte Carlo code for light propagation in sprays and other scattering media, Master Thesis, Lund University, 2011.
[10] Berrocal, E., Multiple scattering of light in optical diagnostics of dense sprays and other complex turbid media, Ph.D. Thesis, Cranfield University, 2006.
[11] van de Hulst, H. C., Light scattering by small particles, Dover, N.Y., 1981.
[12] Bohren, C., and Huffman, D., Absorption and scattering of light by small particles, Wiley, N.Y., 1983.