Monte Carlo method and approaches to simulation of radiation transfer in turbid biological tissues

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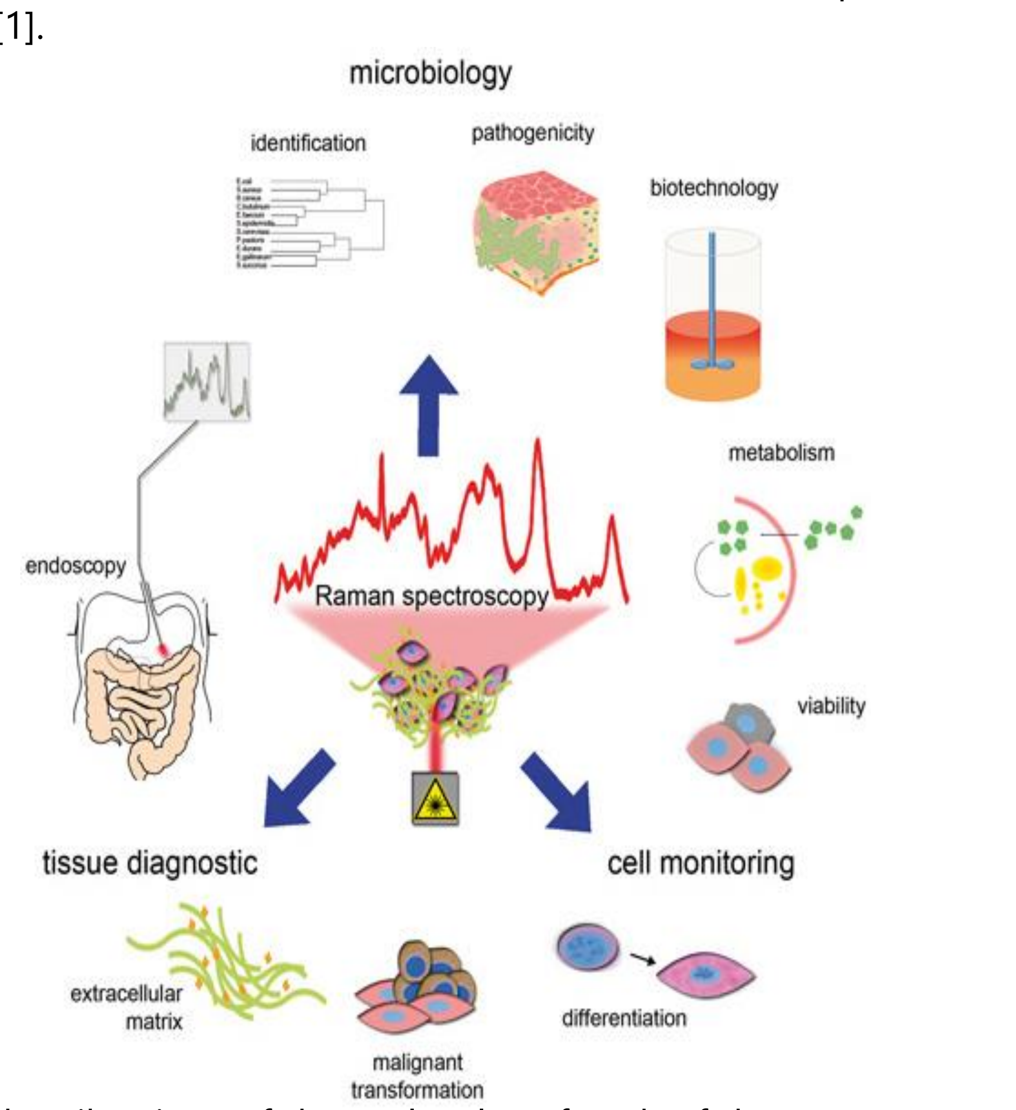
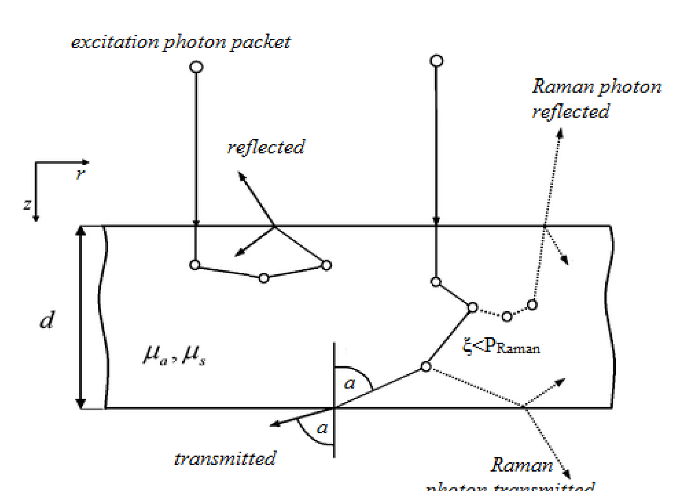
Abstract. Monte Carlo (MC) simulation for light propagation in scattering and absorbing media is the gold standard for studying the interaction of light with biological tis-sue and has been used for years in a wide variety of cases. The interaction of pho-tons with the medium is simulated based on its optical properties and the original approximation of the scattering phase function. Over the past decade, with the new measurement geometries and recording techniques invented also the corresponding sophisticated methods for the description of the underlying light-tissue interaction taking into account realistic parameters and settings were developed.

- Analysis of biological tissues using light-induced optical signals is widely used for various medical, diagnostic and therapeutic purposes.
- One of the tools for molecular optical analysis is confocal Raman microscopy, which makes it possible to detect inelastically scattered photons in a medium. These photons have a shift in wavelength relative to the radiation that excites them. The energy difference for each inelastically scattered photon corresponds to the molecular structure of a certain sample under study [1].



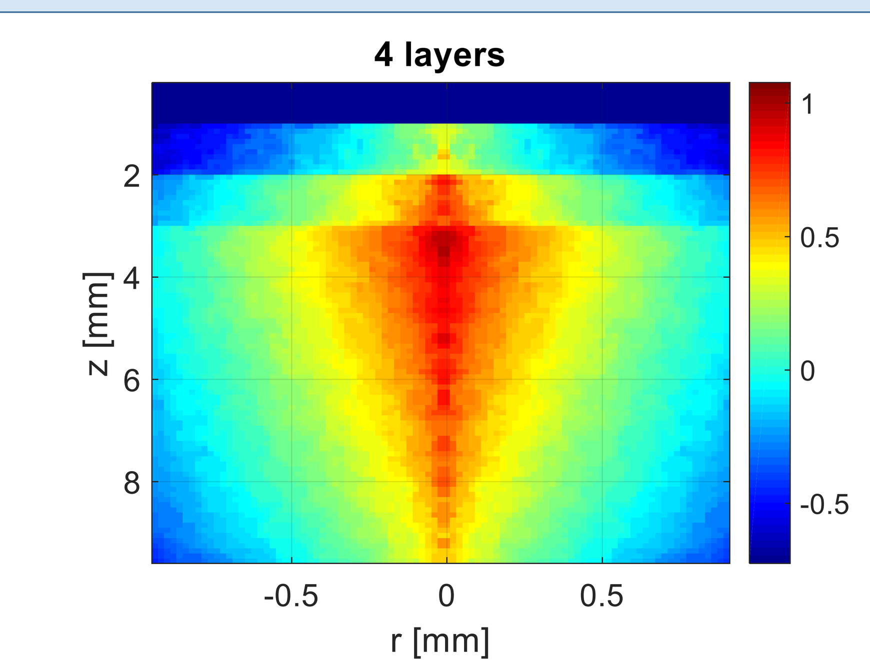
- Thus, the vibrations of the molecules of each of the components produce a characteristic Raman spectrum or a kind of "fingerprint" that can be used to determine the chemical and structural composition of the sample [2].
- To date, there are two main reasons why the problem of reliable quantitative determination of the attenuation of the Raman signal cannot be satisfactorily solved: the lack of adequate models and reliable modeling tools, on the one hand, and insufficient knowledge about the effect of optical properties and distribution of scatterers in the sample, on the other hand. another [3 - 5].

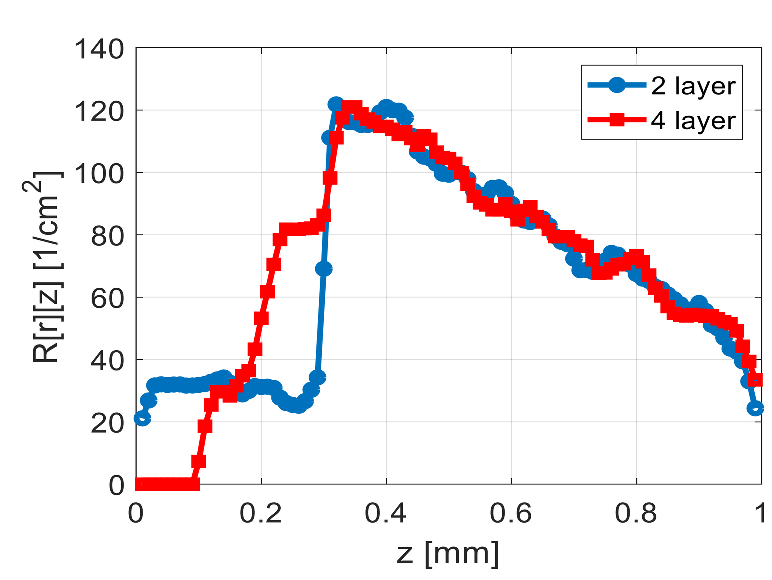
General scheme of the MC model for Raman



- At each step (circles), part of the photons from the photon packet is absorbed.
- The solid lines show the trajectories of elastically scattered photons, the trajectories of Raman scattered photons are shown as dotted lines.
- The depth of the medium is z, r is the radial coordinate.

From optical imaging, one can now expect the same breakthrough in the field of non-operative diagnostic methods that was provided by X-ray and computed tomography at that time, thanks to the use of non-ionizing radiation and its non-invasiveness [3]. Diffuse reflectance spectroscopy (DRS), near infrared spectroscopy (NIRS), diffractive optical tomography (DOT), Raman tomography, fluorescence tomography, optical microscopy, optical coherence tomography (OCT) and photoacoustic (PA) imaging are among the most widely used in modern times. optical methods in biomedicine, and their potential is far from fully understood [4-5].
The modeling of light propagation in a medium is based on the absorption and scattering characteristics that dominate the propagation of light in biological tissues. The usual approach to modeling the propagation of light in a medium is to use the radiative transfer equation (RTE). Effective solutions or approximations of this equation for a heterogeneous medium (tissue) are still an open question [6-8].
Modeling the propagation of light in biological tissue based on the MC method has become an important tool for understanding the intricacies of the interaction of light with matter in complex environments. In addition to efficient algorithms, the approximations underlying the model are the key to recent advances in this field. An intensive re-search is currently underway to develop more comprehensive yet effective modeling tools that cover all aspects of the system itself, as well as take into account all relevant environmental influences [8]. In addition, the trend indicates the use of more anatomically realistic geometries and the development of more user-friendly modeling tools. The further development of biophotonics lies in the ever-increasing processing power of computing systems and artificial intelligence concepts such as the concepts of machine learning, deep learning and data analysis.





Depth-resolved distribution of absorption probability of reemissed Raman photons in the 4-layer bCar+ink solution (top). Simulated Raman photon fluence (bottom)

Summary

The MC based simulation of light propagation in biological tissue has emerged to an important tool for understanding the subtleties of the light-matter interaction in complex media relevant to the fields of medicine and the life sciences, for example. Apart from efficient simulation algorithms accurate modeling is the key for the recent advances in the field. New insights obtained from the simulations serve as valuable input for the design of novel instruments based on non-invasive, optical principles or facilitate the interpretation of measured data obtained from bio-logical samples. The simulation methods presented in this review are mainly focused on biomedical optical imaging and spectroscopy. However, they will likely influence further fields of application in the near future. Consequently, intense research is currently under way to develop more comprehensive and at the same time efficient simulation tools taking into account all aspects of the system itself as well as incorporating all relevant environmental influences. Also, the trend points towards the use of anatomically more realistic geometries and the development of more user-friendly simulation tools. As the field is already undergoing the translation from basic research to practical applications, for example, in clinical environments or in the field, a large variety of optical systems with enhanced functionality are expected to evolve in the mid and long term. Further benefit will be generated by the ever increasing computing power available and artificial intelligence concepts such as machine learning and deep learning concepts which will likely also advance modeling and simulations as well as data analysis.

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