# Skin color simulation - review and analysis of available Monte Carlo-based photon transport simulation models

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## Abstract

*Optical assessment is a useful tool for non-invasive skin assessment avoiding scarring, time delayed diagnosis, hurting, and inconvenience for patient and practitioner. This has led to wide adaption of digital imaging and other optical technologies in dermatology. Many of these optical technologies lack quantifiability, therefore, the reproduction, comparison or absolute meaning of measurements or images is an open challenge. Monte Carlo simulation for multi-layered turbid media provides an accurate tool for simulating the optical path of photons traversing in the skin and the diffuse spectral reflectance of skin. With this tool at hand the missing link between health metrics and measurable optical phenomena can be provided and it can help to establish optical assessment and digital images as a standard for health monitoring of skin. A number of publicly available simulation codes and several different approaches have been proposed. In this work we give an overview of three Monte Carlo simulation tools and compare the different approaches. Furthermore, we will use Monte Carlo Simulations to generate different spectra based on varying optical properties and use these spectra to generate colour patches to analyse the impact of different optical properties on the resulting RGB colour patches.*

## Introduction

Useful health information with a minimal impact for the patient can be achieved through optical techniques. Common optical techniques for skin assessment are diffuse reflectance spectroscopy [1–3] and standard RGB sensors [4–7]. Quantifiability of these medical skin imaging or optical health assessment technologies is an open challenge. Several approaches to obtain more reliable and quantifiable results are based on photon simulation in tissue [8–15]. Next to the bio medical field optical skin simulation has been applied in the computer graphics community in order to generate realistic looking skin. The complexity of the models used has been gradually increasing incorporating and taking into account more physiological properties. Nevertheless the impact of tresearch in the computer graphics community did not have a big effect on the bio medical sector [16]. Many of the techniques are based on diffusion theory [17].

Also some proposed techniques for the simulation of tissue light interaction in the bio medical field are based on diffusion theory [3, 15] or and many on Monte Carlo sampling [8, 12, 18]. Diffusion theory is only applicable under the assumption that the scattering dominates over absorption [3] and is limited for thin layers. It is computationally efficient and can provide results in near real time [19].

Monte Carlo simulation on the other hand is considered to provide accurate [9] results of tissue light interactions unrelated to the thickness of the layers. It is a sampling technique allowing an accurate description of light transport over a wide range of length scales. This can be performed in absence of a complete analytic model due to statistical sampling. Each photon is hereby simulated with an energy level and moved through the predefined medium interacting with it based on optical parameters and statistical sampling. The photon energy decomposition and its directionality are preserved. Simulation provides insights into complex light tissue interactions including photon path length traveled, depth sensed, spectral response and others. It allows investigation of the influence of optical properties which can be difficult or impossible to control. Publicly available implementations of Monte Carlo simulation have been used in recent years [8, 12]. Wang *et al.* [12] proposed a versatile publicly available C implementation in 1995, which has found great attention in the scientific community and resulted in many studies [8–10, 13]. New implementations of Monte Carlo simulation have emerged and are making use of the graphics processing unit (GPU)in modern computers. One example of such a code is the GPU based MCX code by Fang *et al.* [8]. Fang's implementation is based on the same general principles but is designed to be executable on modern GPUs which allows the calculation of multiple photons at the same time speeding up the simulation process significantly.

In this study we compare different implementations of Monte Carlo simulation for skin. Namely the MCML (Monte Carlo for multi-layered media) by Wang *et al.* [12], MCXYZ (3D Monte Carlo) for heterogeneous tissue code published by Jacques *et al.* [20] and the MCX Monte Carlo extreme implementations including MMC (mesh based Monte Carlo) by Fang *et al.* [8] We will compare the simulation results and give insights on how to use the different Monte Carlo simulation codes for simulating diffuse spectral reflectance of skin. These simulated spectra will be used to generate color and the influence of different parameters onto the final color patches will be compared. They can give information about the relationship between skin color and health relevant chromophore concentrations and the impact of underlying pathologies or structures onto the skin color. Furthermore, the generated images can illustrate the impact of different light sources used for skin imaging and its influence on the final color image.

## Background

### *Skin optical properties*

In the following section we discuss general skin optical properties based on the book by Wang *et al.* to give an overview of the

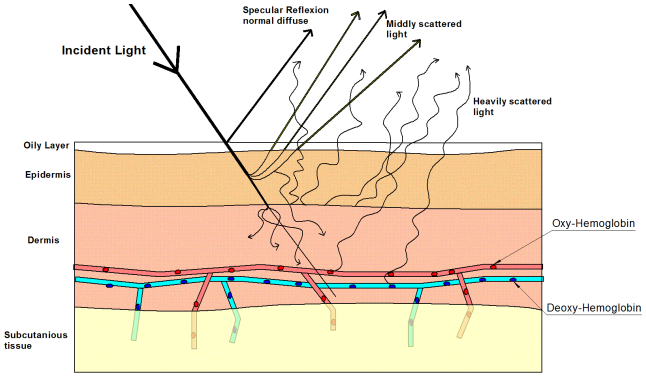


***Figure 1.*** *General skin structure and simplified interaction of skin and radiation. Figure reproduced from Bauer [22].*

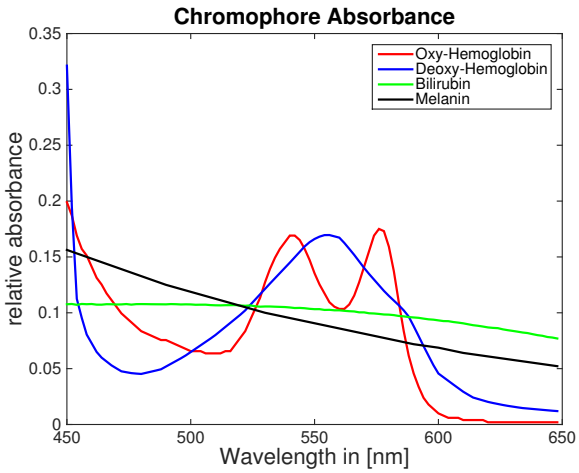


***Figure 2.*** *Optical absorption spectrum of common chromophores in human skin data from Jacques* et al. *[23]*

relevant parameters for optical skin simulation [21]. The interaction of light and tissue is mainly based on scattering and to a significantly smaller degree on absorption. The absorptions is especially weak in the 400-1350nm spectral region and the mean free path between photon scattering events is on the order of 0.1mm compared to the mean absorption path length in the order of 10-100nm. In order to simulate skin we have to define optical properties and formulate a general model describing the skin structure. As a simplification skin can be described as a three layer model with three main layers defining different areas of optical properties. These layers are usually the epidermis, dermis and the subcutaneous tissue from the outside to the inside of the skin. Figure 1 shows the simplified light tissue interaction we use for the definition of our input tissue structure for simulation. Absorption plays a significant smaller role compared to scattering events for light simulation. The absorption can be described as:

$$I_0/I = -\mu_a dx, \tag{1}$$

where x denotes the distance traveled of the light, $I_0$ denotes the incoming light and $I$ the outcoming light in a set up where light is incident to a medium and the resulting light on the other side is measured. The equation describes the proportionality percentage of the light absorbed in the interval (x,x+dx) to the product of $\mu_a$ and dx. This is usually formulated in the well known Beer Lambert law as:

$$I(x) = I_0 e^{-\mu_a x}. \tag{2}$$

Specific components in the skin the so called chromophores can be considered the main absorbers in skin and are of interest for skin and general health assessment. Figure 2 shows the absorption coefficients of the most common chromophores in biological tissue per wavelength. These absorption curves can then be used to define the total absorption of the different skin layers with varying concentrations of the different chromophores. The optical properties are mainly governed by scattering in the tissue. To describe the scattering properties we define the scattering coefficient $\mu_s$ as the probability of photon scattering in a medium per unit path length [21]. This leads to Beer's law describing the probability of a photon propagating distance x without a scattering event,

$$T(x) = e^{-\mu_s x}. \tag{3}$$

T(x) is hereby the ballistic transmittance and $\mu_s$ the reduced scattering coefficient. The scattering is strongest for biological structures with a size which matches the optical wavelength of the photon, therefor the scattering is wavelength dependent. Another important property for optical skin simulation is the so called anisotropy factor g. This factor is defined as the $cos(\Theta)$ with values from -1 to 1. $\Theta$ describes the angle of the scattering direction and $g = 0$ corresponds to isotropic scattering and 1 dominantly forward scattering and correspondingly -1 dominantly backward scattering. In biological tissue the anisotropy factor is usually 0.9 so mainly forward scattering [21].

The last important quantity for Monte Carlo simulation is the fluence rate $F$. Fluence rate $F$ measured in $\mathrm{W/cm^2}$ is commonly the output of Monte Carlo simulation tools. It refers to the irradiance which is incident from all angles onto a small region of space [23]. This is used for turbid media where light is scattered towards the target from all directions. It describes the total irradiance impinging onto a target region from all directions. The fluence rate $F$ is the power absorbed by that region, $P_{absorbed}$, divided by its cross sectional area, $A$ (total area of the light cross section):

$$F = P_{absorbed}/A. \tag{4}$$

In the case of a small region the fluence rate is independent on the size of the region and depends on the primary plus secondary irradiance impinging onto that region.

## Skin simulation

The simulation requires the definition of skin optical properties, specific structures and the user choices of simulation parameters. Simulation parameters include: number of photons, volume (input structure), properties (optical properties of the structure usually $\mu_s, \mu_a, n, g$), $t_{start}, t_{step}, t_{end}$ or the duration of the simulation, source position, source direction, type of source. In the cases discussed in this paper the input structure is a 2D structure a 3D cube or mesh grid. Each layer, voxel or triangle respectivel is associated to optical properties defined as an input variable for the simulation. The absorption $\mu_a$ is calculated as a combina-

tion of several parameters including the blood concentration with oxygenated hemoglobin and deoxygenated hemoglobin, melanin concentration, and water concentration. It is then calculated with the following formula:

$$\mu_a = B*(S*\mu_a(\lambda)_{oxy}+(1-S)*\mu_a(\lambda)_{deoxy})+ W*\mu_a(\lambda)_{wat}+M*\mu_a(\lambda)_{mel}) \quad (5)$$

In which B denotes the total blood concentration S denotes an oxygenation saturation and W and M correspond to the melanin and water concentrations. Depending if the voxel belongs to the dermis or the epidermis these values vary. In healthy skin we would not expect the majority of melanosomes in the epidermis and only a small amount of oxy- and deoxyhemoglobin in the epidermis [24]. Equally we would expect a small concentration of melanin in the dermis and a higher concentration of blood including oxy- and deoxy-hemoglobin in the dermis. Additionally areas with for example increased melanin concentration could be defined and correspond for example to a mole in the epidermis.

The next parameter which has to be defined is the $\mu_s$ reduced scattering coefficient. Jacques [25] proposed a formula which has been used extensively in the domain of skin simulation to calculate the scattering coefficient wavelength dependent.

$$\mu_s'(\lambda) = a'(f_{ray}(\frac{\lambda}{500nm})^{-4}+(1-f_{ray})(\frac{\lambda}{500nm})^{-b_{mie}}) \quad (6)$$

To obtain a dimensionless equation dependent on the wavelength it is normalised and divided by the reference wavelength at 500nm. The factor $a\prime$ is the $\mu_s(500nm)$ scattering coefficient at 500nm. Wavelength dependence is then described separately for its Rayleigh scattering contribution and its mie scattering contribution. All the different simulation algorithms examined in this paper require the definition of these structures priori to run time.

Monte Carlo simulation of photon transport follows this simulation pattern or concept. Each photon has an initial amount of energy and is propagated in a direction. In the beginning this direction is defined by the user input parameters for the $x_{focus}, y_{focus}$ and $z_{focus}$. Each photon is then moved a specific step forward in case the photon crossed a boundary it is either reflected or transmitted in the case it did not cross a boundary it will be absorbed or scattered. The absorption properties of the medium define the amount of energy absorbed by the corresponding voxel. Scattering properties and Monte Carlo sampling define the new direction of the photon. As the last step of one iteration the photon depending on the energy left and a random roulette is either terminated or it will go through the whole cycle again. This whole process is continued until the last photon died which terminates the algorithm.

**MCML** Monte Carlo for multi layered media (MCML) is a Monte Carlo simulation code which has been publicly available since 1995 and was released by Wang *et al.* [12] [23]. It has been used by many research groups in the past years some examples are it was utilised to generate lookup tables providing the link between diffuse spectral reflectance and chromophore concentrations in phantoms by Hennesy *et al.* [26], to obtain look up tables for a multiple regression approach to obtain melanin and hemoglobin concentration by Nishidate *et al.* [13] , it has been extended to consider 3D structures in skin by Paquit *et al.* [27] and Naglic *et al.* combined MCML with diffusion theory to get health information from diffuse spectral reflectance [10]. The model on which MCML is based on considers multilayered skin as infinte wide layers parallel to each other. Light is introduced to this structure perpendicular to these layers. MCML works in a cylindrical space with a radial coordinate system assuming an indefinite expansion if the optical properties provided to the model. It is build to simulate the photon transport through these media and considers photons as particles therefore polarisation and wave properties are neglected.

Table 1 shows the input properties for the MCML code. The optical properties of the layers $\mu_s, \mu_a, n, g$ can then be calculated from given blood, melanin and oxygen saturation values according to the formulas discussed in section .

**MCXYZ** Monte Carlo XYZ indicating the dimensionality of the model (MCXYZ) is a C code provided by Jacques *et al.* [23] it is designed to work with 3D cubes which are composed of 3D voxels. It is provided including two Matlab scripts allowing the preparation of the input file and the viewing of simulation results. In order to use the code several paramaters have to be defined with some variations compared to general Monte Carlo parameters. Most of them are inherit to the architecture of the tissue definition. Defining the optical properties can be considered as the definition of a palette of tissue types each tissue type gets an integer identifier 1-19 and its optical properties $(\mu_s, \mu_a, g)$. These can then be used to define the 3D structure which contains a 3D cube with the corresponding tissue type identifier. The Matlab file maketissue.m can be used to define different tissues by creating shapes inside the defined cube. MCXYZ can then be used to simulate the light tissue interaction with the input structure.

**MCX** Another Monte Carlo simulation tool we will consider is the Monte Carlo extreme (MCX) implementation being the most recent implementation by Fang *et al.* [8] it is completely parallelised and optimised to run on a GPU. Parallelisation and GPU processing can speed up the Monte Carlo simulation significantly, since each photon can be treated individually and many photons can be processed simultaneously. This speeds up the simulation time by a factor of 300 or more, depending on the computing power of the GPU used [8]. Due to the different implementation MCX also requires some additional input variables compared to the unparellised mcml and MCX described in section . The MCX code follows a similar concept to the MCXYZ code based on a cubic voxel grid, where each element has optical properties assigned to it. General functionality is close to MCXYZ but it provides a lot more flexibility for the user to define the input lightsource. Additionally it runs significantly faster to the unparallelised MCXYZ code. This comes of course with the necessity of a CUDA capable graphics card to use this implementation.

**MMC** Fang also proposed MMC a mesh based Monte Carlo simulation code. This code is not parallelised (at the time of writing of this paper) for a GPU but it is the principles are the same to the MCX code. The main difference between MMC and MCX is the input structure definition since, it is based on a mesh definition of the input structure. So to define the tissue structure it requires nodes for a tetrahedral mesh grid and an element ar-

**Table 1: Monte Carlo methods predefined variables**

| General Monte Carlo | MCML | MCXYZ | MCX |
|---|---|---|---|
| number of photons | input file | determined by simulation time | defined as input |
| volume (input structure) | just layers considered infinitely wide | 3D voxel integers (1-19) | 3D voxel integers |
| optical properties($\mu_s, \mu_a, n, g$) | input file | list defining tissue 1-19 | list defining tissue |
| simulation time | determined by number of photons | total simulation time defined | $t_{start}, t_{end} t_{step}$ |
| source position | on top of the tissue | x,y, z, coordinates | x,y, z, coordinates |
| source direction | perpendicular to tissue in z(depth) | $x_{focus}, y_{focus}, z_{focus}$ | $x_{focus}, y_{focus}, z_{focus}$ |
| type of source | infinitely narrow beam | uniform, gaussian, isotropic pt | 14 different types |
| wavelength | defined in input file | wavelength for simulation | wavelength for simulation |
| cuda parameters | none | none | $n_{blocksize}, n_{threads}, seed, max_{gate}$ |
| detector definition | none | none | define locations of detectors |

ray. This allows an even more efficient definition of very thin layers and can result in significant computational efficiency improvements. Furthermore a mesh grid input definition allows for different and more complex structures opposed to the voxel definition of MCXZY.

## Experiments

We have simulated a 3 layer skin structure using the MCML (Monte Carlo for multilayered media). As a proof of concept we chose the implementation and optical properties published by Atencio *et al.* [24]. Atencio *et al.* have used MCML to generate spectra for different concentrations of bilirubin in the dermis region of the skin. We defined the optical properties of the skin and ran the simulations and plotted the resulting spectra with varying bilirubin concentrations in the epidermal layer. Figure 3 shows the results obtained by simulating the different amounts of bilirubin in the dermis region of skin.

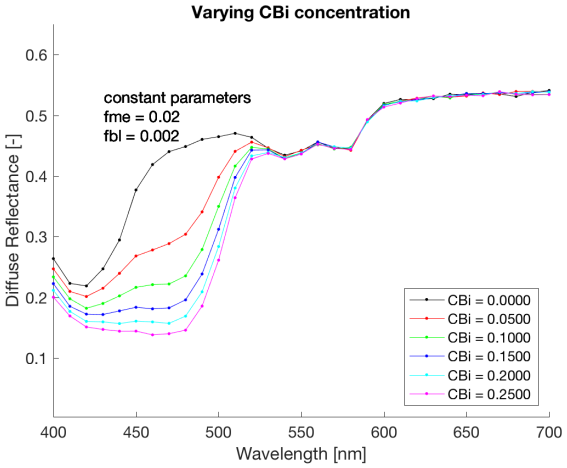


***Figure 3.*** *Different concentrations of bilirubin in the skin simulated spectra using MCML and the configuration proposed by Atencio* et al. *[24]*

We then used these simulated spectra for the generation of colour patches based on Monte Carlo simulations. As a first step we simulated a simple 3 layer model using the mcml implementation discussed in section  and using publicly available Matlab code. The model and the code used for the simulation is publicly available by Atencio *et al.* and discussed in detail in [24]. It is based on a 3 layer model with a thin epidermal layer a hypodermis and a bone layer, this model assumes the measurement on the skull of neonatal babies. The optical parameters mainly the concentrations of different chromophores in the skin for the simulation were varied between the different runs but the structure itself remained unchanged. In order to simulate with different chromophore concentration we had to adjust the publicly available simulation code by Atencio *et al.*, while still keeping the general structure. Three experiments were performed, while changing different chromophores Melanin, Bilirubin and the total blood concentration (haemoglobin). Correspondingly we kept the other chromophore concentrations constant in this experiment. The mcml code was then used to generate diffuse spectral reflectance curves with known chromophore concentrations. In order to simulate colour patches we assumed the mcml resulting spectra, the camera sensitivity curves of a Nikon D300, and in this proof of concept study we used a white LED as the primary lightsource. The sensitivities of the camera were measured prior to this experiment and can be seen in Figure 4.

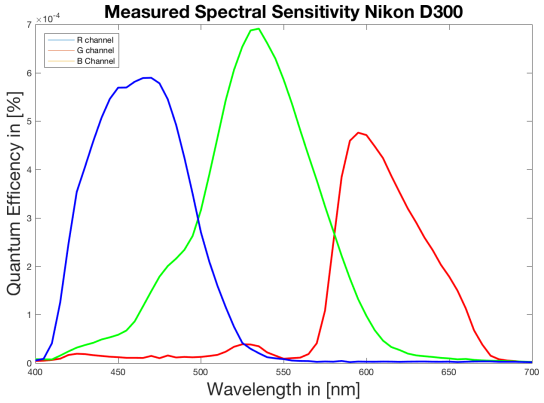


***Figure 4.*** *Measured spectral sensitivities of a Nikon D300*

In figure 5 we plotted different resulting colour patches B1-B6 the numbers under the images indicate the different total blood concentration. We can clearly see the trend of increasing redness depending on the total blood concentration in the model. This agrees well with the expectations for increased blood concentration in the tissue. Due to the optical properties of haemoglobin we would expect a more reddish appearance of the skin. In the next set of simulations, shown in figure 6, we varied the bilirubin. Bilirubin is another chromophore which occurs naturally as a decomposition product of haemoglobin. So commonly we would see higher bilirubin after bruising the skin.

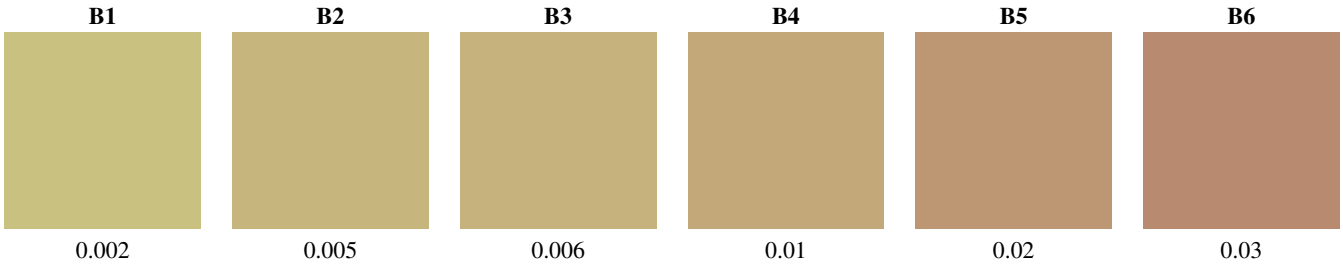


***Figure 5.*** *Colour patches based on Monte Carlo simulations with varying blood concentration as an input variable*

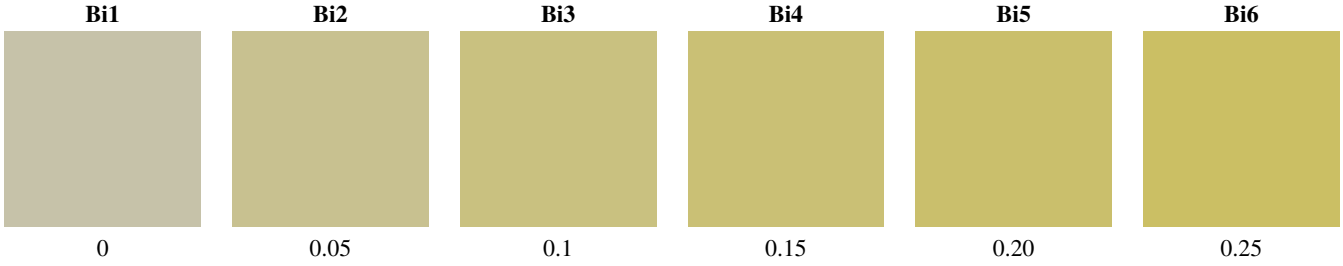


***Figure 6.*** *Colour patches based on Monte Carlo simulations with varying bilirubin concentration as an input variable*

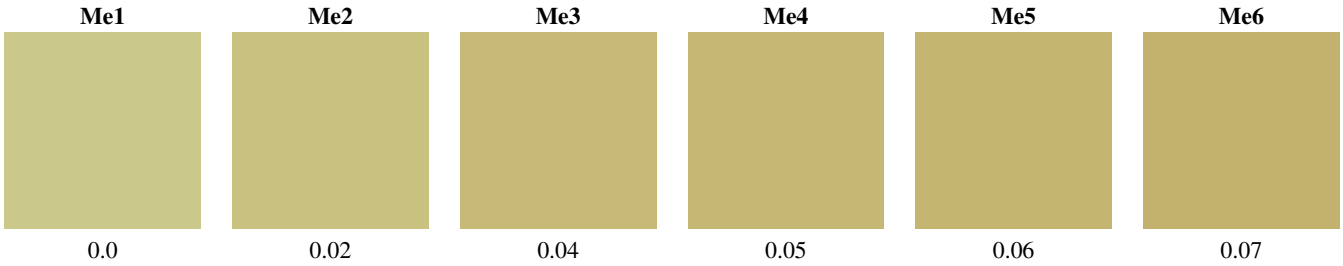


***Figure 7.*** *Colour patches based on Monte Carlo simulations with varying melanin concentration as an input variable*

The results shown in figure 6 also agree well with expectations. A higher bilirubin results in a more yellowish appearing skin. Bilirubin in newborns can be a deadly disorder if not treated accordingly. The detection of bilirubin as soon and as non-invasive as possible is therefore of great importance. We can observe the increasing yellowness in our simulation results very well. In the next experiment we increased the melanin concentration in the epidermal region. Also these results shown in figure 7 agree well with expectations. Melanins with its high absorbance colours the skin in a brown or darker shade. We can observe this colouring in the simulated melanin colour patches.

## Conclusion

MCML assumes a homogenous tissue it provides good results for small skin volumes or for simulating probe measurements. In the case of spatial skin imaging we are especially interested in the inhomogeneous aspects therefore MCML is less suitable. Nevertheless the MCML simulations and the generated skin patches show the expected behaviour.

This paper gives an overview of publicly available Monte Carlo simulation codes and outlines some of their capabilities and limitations. The given codes have been described and differences have been pointed out. Additionally we performed a basic quantitative comparison of the methods by running the different codes with similar input parameters and we are reporting the results. MCX (Monte Carlo extreme) stands out from the implementations discussed since it has the most advanced light source definition, a flexible 3D structure to define the input tissue and has run time and computational efficiency advantages over the other implementations. For very thin layers (like skin) we recommend the MMC implementation, since the runtime should be further decreased by the efficient representation of the input structure in the form of tetrahedral. It comes even more apparent if the author provides a parallelised version of the MMC code. Furthermore we performed an experiment in order to evaluate the usefulness of MonteCarlo simulated spectra for visualising different chromophore concentration levels. As a proof of concept this approach shows good results. All the different chromophores simulated for this study show good agreement with expectations. This could be useful in educational purposes for dermatologists in order to aid to give them a better understanding how depth or general concentration of these chromophores influences the resulting colours imaged by for example a digital three channel sensor. Furthermore, the mechanisms of colour image formation and chromophore concentrations can be further studied.

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## Author Biography

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