Hyperspectral Modeling of Material Appearance: General Framework, Challenges and Prospects

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Abstract: The main purpose of this tutorial is to address theoretical and practical issues involved in the development of predictive material appearance models for interdisciplinary applications within and outside the visible spectral domain. We examine the specific constraints and pitfalls found in each of the key stages of the model development framework, namely data collection, design and evaluation, and discuss alternatives to enhance the effectiveness of the entire process. Although predictive material appearance models developed by computer graphics researchers are usually aimed at realistic image synthesis applications, they also provide valuable support for a myriad of advanced investigations in related areas, such as computer vision, image processing and pattern recognition, which rely on the accurate analysis and interpretation of material appearance attributes in the hyperspectral domain. In fact, their scope of contributions goes beyond the realm of traditional computer science applications. For example, predictive light transport simulations, which are essential for the development of these models, are also regularly being used by physical and life science researchers to understand and predict material appearance changes prompted by mechanisms which cannot be fully studied using standard "wet" experimental procedures. For completeness, this tutorial also provides an overview of such synergistic research efforts and *in silico* investigations, which are illustrated by case studies involving the use of hyperspectral material appearance models.

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1 Introduction

Material appearance models are integral components of image synthesis pipelines. Through these models, one simulates how different materials reflect and transmit light so that they are assigned appropriate appearance attributes such as color, glossiness and translucency. Undeniably, significant progress has been achieved in this area [37]. We have moved from physically-inspired to physically-based models, and the impact on the realism of computer generated images has been remarkable. In fact, the current rendering technology allows the generation of believable images of a wide range of materials, especially man-made ones, which are in many instances indistinguishable from their real counterparts.

More recently, substantial efforts have been directed toward the development of models that can be used to generate images that are not only believable, but also predictable. Accordingly, the motivation for this tutorial lies in the central role played by predictive material appearance models in realistic image synthesis, and in the timely opportunities that their development offers for expanding the frontiers of research across different fields. Arguably the exploration of the hyperspectral domain, spanning from the ultraviolet (UV) to the infrared (IR) regions of the light spectrum, represents one of such frontiers leading to a host of new educational, creative and scientific applications [29, 66].

In order to develop predictive hyperspectral models, a scientifically sound methodology, involving data collection, model design and evaluation, should be employed. Hence, in this tutorial, we examine the practical constraints that that need to be addressed in each of these stages of the model development framework (Figure 1). For completeness, we also address performance and reproducibility issues that can hinder the usability of these models. Finally, we employ case studies to show that the pursuit of model correctness is an iterative process, which itself can contribute to accelerate the hypothesis generation and validation cycles of research in different fields.

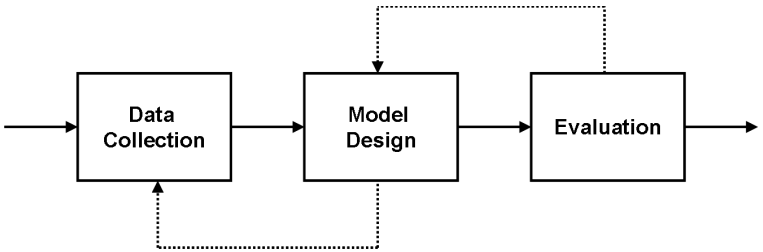

Figura 1. Diagram depicting the three main stages of the model development framework and its iterative nature, with feedback information (dotted lines) potentially prompting refinements in all stages.

2 Biophysical Background

In this section, we briefly outline concepts and terminology employed in this tutorial. The reader interested in their detailed descriptions is referred to more comprehensive texts on related topics (*e.g.*, [8, 19]).

2.1 Light Interactions with Matter

The appearance of a given material is directly dependent on its interactions with light. Among the myriad of phenomena encapsulated by these interactions, emission, scattering and absorption are known to have the largest impact on material appearance. For this reason, these phenomena are concisely described in this section.

Man made and natural light sources emit light with characteristic spectral distributions, which depend on the nature of the emission process. The processes of light emission can be divided into two main types: thermal and luminescent [2, 65]. Thermal emissions are due to the material radiating excess heat energy in the form of light. In the case of luminescent emissions, energy arriving from elsewhere is stored in the material and reemitted after a short period of time.

The term scattering refers to the deflection of light through collisions with molecules, particles (an aggregation of sufficiently many molecules) or multiple particles. Besides the change in direction, the energy of the incident light may also be weakened (attenuated) in the process. The main types of scattering occurring in Nature are Rayleigh scattering, Mie scattering and reflective-refractive scattering.

Rayleigh scattering [110] occurs when the wavelength of the incident light is somewhat larger than the molecules or particles. This type of scattering is proportional to the fourth power of the frequency, *i.e.*, the shorter wavelengths are preferentially attenuated. Mie scattering [80] occurs when the wavelength of the incident light is comparable to the size of the molecules or particles. Finally, reflective-refractive, or geometrical optics, scattering occurs when the size of the particles is much larger than the wavelength of incident light.

Materials such as conductors (metals), semi-conductors and dielectrics are characterized by their complex index of refraction, which is composed of a real and an imaginary term. The real term corresponds to the real index of refraction, also called refractive index, which measures how much an electromagnetic wave slows down relative to its speed in vacuum [114]. The imaginary term corresponds to the extinction index, also called extinction coefficient, which represents how easily an electromagnetic wave can penetrate into the medium [114].

The reflective-refractive scattering accounts for most of the internal light deflections

occurring within organic tissues and particulate materials. Due to its dependence on refractive differences, the variations across the spectrum are directly associated with the spectral profile of the materials' refractive indices (Figure 2 (Left)).

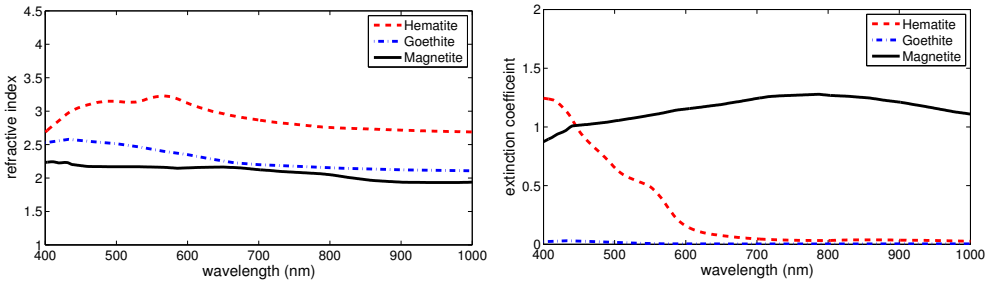

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Figura 2. Spectral data for iron oxides commonly found in sandy landscapes: hematite [107], goethite [39] and magnetite [104]. Left: refractive index (index of refraction, real term). Right: extinction coefficient (index of refraction, imaginary term).

Once light is transmitted into a medium, it may be absorbed. In a dielectric, this may happen if there are absorptive elements, such as pigments and dyes, inside the medium. Pigments are materials that exhibit selective scattering and selective absorption, while dyes exhibit selective absorption and some luminescence produced due to excitation [43]. The resulting spectral distribution of light going through an absorption process depends on the absorption spectrum of the absorptive element.

The absorption spectra of pigments, such as chlorophyll, melanin and hemoglobin, are usually given in terms of their specific absorption coefficient (s.a.c.). This quantity can be obtained through direct measurements, or by dividing the material's molar extinction coefficient by the material's molecular weight. Its units depend on how the concentration of the material is measured. In the case of inorganic materials (*e.g.*, water and iron oxides), the absorption spectra is usually given in terms of their extinction coefficient (Figure 2 (Right)). The s.a.c. of these materials can be obtained by multiplying their extinction coefficient by the ratio $4\pi/\lambda$, where λ represents the wavelength of light [22].

2.2 Applied Optics Terminology

A level of abstraction commonly employed in applied optics simulations consists in describing materials as random turbid media with volumetric scattering and absorption properties [96]. These properties are represented by the volumetric absorption and scattering coefficients. Since the term volumetric is usually omitted in the applied optics literature, for the sake of consistency, we will also omit the term volumetric throughout this document.

The absorption coefficient is obtained by multiplying the density of a material's absorbers (absorbing particles) in the medium by the absorption cross section of an individual absorbing particle [57]. The absorption cross section, in turn, corresponds to the total power absorbed by the particle, and it is a function of the particle's orientation and the incident light's state of polarization [119].

Similarly, the scattering coefficient is obtained by multiplying the density of a material's scatterers (scattering particles) in the medium by the scattering cross section of an individual scattering particle [57]. The scattering cross section, in turn, corresponds to the total power scattered by the particle, and it is also a function of the particle's orientation and the incident light's state of polarization [119].

The sum of scattering and absorption coefficients gives the attenuation coefficient. In applied optics these coefficients are usually used to describe the optical properties of whole materials instead of their basic constituents. This approach may introduce undue inaccuracies in simulations of light propagation in organic tissues since these coefficients are usually determined by inverting light interaction models whose correctness may not have been properly evaluated in the first place.

Three other parameters are commonly used to simulate light propagation in a material assumed to be a random medium with volumetric properties: albedo, optical depth and phase function. The albedo is a dimensionless parameter defined as the ratio between the scattering coefficient and the attenuation coefficient. The optical depth represents the product of the tissue thickness and the attenuation coefficient [96]. Finally, a phase function describes the amount of light scattered from the direction of incidence to the direction of scattering [119].

2.3 Measurement of Appearance

The group of measurements necessary to characterize both the color and surface finish of a material is called its *measurement of appearance* [56]. These measurements involve the spectral and the spatial energy distribution of the propagated light. While, variations in the spectral distribution of the propagated light affect appearance characteristics such as hue, lightness and saturation, changes in its spatial distribution affect appearance characteristics such as glossiness, reflection haze, transmission haze, luster and translucency.

The spectral energy distribution of the propagated light is usually measured in terms of reflectance and transmittance [86]. The reflectance can be defined as the spectral power distribution of the reflected light, *i.e.*, the ratio of the reflected flux to the incident flux (Figure 3). Similarly, transmittance represents the spectral power distribution of the transmitted light, *i.e.*, the ratio of the transmitted flux to the incident flux. The light that is neither reflected nor transmitted by the materials is absorbed. The parameter that describes the amount of absorbed light is absorptance.

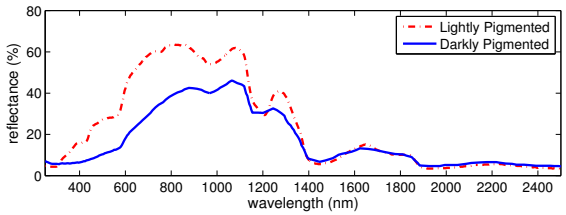

Figura 3. Reflectance spectra for lightly and darkly pigmented skin specimens provided by Cooksey and Allen [31] and Jacquez *et al.* [62, 61], respectively.

The spatial patterns of light distribution are represented by the bidirectional scattering-surface distribution function (BSSDF) [86]. This function is considered to be difficult to measure, store and compute due to its dependence on four parameters: the incidence and outgoing directions, the wavelength and the position on the surface. For this reason, sometimes it is more practical to make simplifying assumptions about the material in order to obtain a more tractable function, and still obtain a useful degree of approximation for the cases of interest [86]. For example, if one assumes that the scattering properties of a given material are uniform, the dependence on the location of the point of observation (reflection) can be omitted [86]. In this case, one can work with a simpler function, namely the bidirectional scattering distribution function (BSDF, or simply BDF), which can be decomposed into two components: the bidirectional reflectance distribution function (BRDF) and the bidirectional transmittance distribution function (BTDF).

3 Quest for Predictability

A predictive model is capable of providing high fidelity results obtained through simulations controlled by biophysically meaningful parameters. Fidelity, in this context, corresponds to the degree to which a model reproduces the state of a real world object in a measurable manner, *i.e.*, a measure of its realism and faithfulness [47]. In other words, the correctness of the modeled results needs to be evaluated through quantitative and qualitative comparisons with measured data.

The use of predictive appearance models makes the image synthesis process less dependent on ad hoc tweaks, allowing for a more automatic replication of the modeled results. Once it can be demonstrated that the predictions of a given model are correct, its scope of applications can be extended beyond the rendering of believable images [46]. For example, predictive models of light interaction with organic layered materials, such as human skin, can be used not only in computer graphics applications involving the generation of realistic images of virtual characters (*e.g.*, [8]), but also in pattern recognition, computer vision and

image processing investigations aimed at the screening of medical conditions (*e.g.*, [4, 6, 27]), the reconstruction of facial features (*e.g.*, [50, 92, 109]) and the remote detection of human signatures during search and rescue operations (*e.g.*, [3, 40, 89]), just to name a few.

Similarly, models of light interaction with inorganic particulate materials, such as sand, can be used not only in the generation of images depicting the appearance of landscapes (*e.g.*, [68, 69]), but also in the remote hyperspectral analysis of their morphological attributes and mineral content (*e.g.*, [10, 11]). In the case of artistic objects and historic documents, their conservation can be substantially enhanced through the use of hyperspectral imaging analysis algorithms supported by predictive material fading simulations (*e.g.*, [51, 67, 70, 90]).

In order to achieve predictability, three main "ingredients" are required: biophysically-based approaches, interdisciplinary efforts and scientifically sound (model) development frameworks (Figure 1). In the remainder of this document, we will address the interplay and the importance of these ingredients.

4 Data Collection

It is a well known fact that a well designed model is of little use without reliable supporting data. This can be classified into three main types: biophysical data (*e.g.*, refractive indices and absorption coefficients) and specimen characterization data (*e.g.*, thickness and pigment concentrations) to be used as input, as well as evaluation data (*e.g.*, spectral reflectance and transmittance) to be used in the assessment of its correctness (Figure 4). Although one may assume that this supporting data is readily available, specially for ubiquitous materials such as plants, human tissues and soils, in reality, this is not case. In fact, a common constraint shared by all types of data required by a model is scarcity. In this section, we provide examples to illustrate the magnitude of this problem, and we also examine other major constraints related to the gathering of reliable supporting data.

4.1 Biophysical Data Constraints

Two of the quantities most widely used in light transport simulations are refractive indices and absorption coefficients. Ideally, one would like to have these quantities provided as a function of the wavelength of light, and with respect to a broad region of the light spectrum. In the case of refractive indices, however, the values available in the literature for complex materials formed by different constituents (*e.g.*, plant or human tissues) usually refer only to a single, averaged, value. Although, one could potentially derive the refractive index of these materials using formulations like the Dale and Gladstone law [115], this would require the knowledge about the refractive indices of the material constituents. For example, in the case of a biological tissue like human skin, these would be represented by cells, organelles and

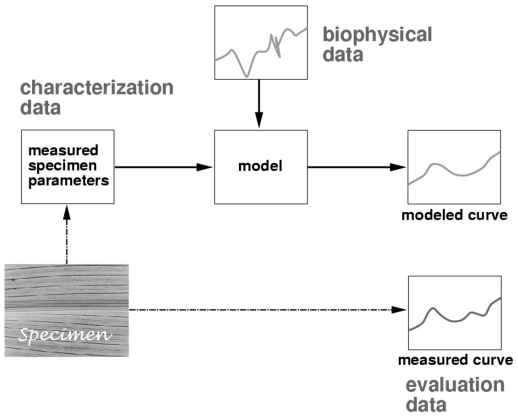

Figura 4. Diagram depicting the main types of data employed in the development of a predictive material appearance model, namely biophysical data (*e.g.*, specific absorption coefficients and refractive indices), characterization data (*e.g.*, thickness and pigment contents) and evaluation data (*e.g.*, reflectance and transmittance curves). Note that ideally the characterization data and the evaluation data should be obtained from the same specimen.

fibers. This data, notably for organic materials, is often not available either. In the case of pure organic materials, it is also worth noting that although their refractive indices are more readily available, often one has to choose between apparently conflicting values for the same material. These discrepancies can also be observed in their extinction coefficients, even for widely used materials like water [48, 91, 94].

When light traverses a turbid medium, refractive index differences between pigment-containing structures and the surrounding medium may cause multiple interactions that increase the light optical path length, a phenomenon known as detour effect [25]. Conversely, the traversing light may undergo a sieve effect, *i.e.*, it may not encounter a pigment-containing structure [75]. While the former increases the probability of light absorption by the pigment of interest, notably in bands of absorption minima, in comparison with a homogeneous solution with equal concentration of this pigment [25], the latter reduces the probability of light absorption, particularly in bands of absorption maxima [75]. The net result of these effects depends on the absorption spectra of the pigments as well as the distribution and volume fraction of the pigment-containing structures (*e.g.*, chloroplasts, melanosomes and red blood cells containing chlorophyll, melanin and hemoglobin, respectively) found in a given material [25, 75].

In the case of specific absorption coefficients for pure materials like chlorophyll or melanin, although one can find data in the literature, it usually corresponds to measurements performed under *in vitro* conditions. However, when one wants to model the appearance of a living material such as a plant leaf or human skin, it is essential to account for the interactions of light with the material constituents under *in vivo* conditions, *i.e.*, including the possibility of detour and sieve effects. These effects, however, are overlooked when absorption coefficients are measured using *in vitro* procedures involving the pigment extraction from the parent material (*e.g.*, chlorophyll extracted from a plant leaf) and in its dissolution using reagents that may also cause spectral shifts in its absorption profile [59].

Absorption data is also often derived through model inversion procedures, which, as outlined earlier, may be biased by the inaccuracies of the inverted model. Moreover, these procedures lack the specificity to allow the distinction between variations of the same pigment occurring in a given material (*e.g.*, different types of chlorophyll found in plant leaves). Techniques based on photoacoustic spectroscopy [103] usually enable such a distinction. However, they provide relative values whose scaling may not be straightforward [41].

4.2 Characterization Data Constraints

In order to correctly simulate the interactions of light with a given material, one also needs to account for its morphological and photobiological attributes. Examples of the former include the thickness of organic tissues as well as the dimensions and shape of material constituents (*e.g.*, sand grains, melanosomes and red blood cells). Examples of the latter include the relative contents of different light attenuation agents (*e.g.*, pigments and water) present in the material. Although it is possible to find ranges for these parameters in the literature, the bounds for these ranges may vary considerably from one bibliographic reference to another.

From a model evaluation perspective, the specimen's characterization data to be used as input should correspond to the specimen on which the reference measurements were performed (Figure 4). However, the relatively few spectral radiometric datasets available in the literature rarely provide a detailed description of the morphological and photobiological attributes of the specimens used in the measurements. One noteworthy exception is the database known as LOPEX (Leaf Optical Properties Experiment) [54].

The LOPEX project involved leaf optical experiments performed on 120 leaf samples representative of more than 50 species. These experiments included spectral curves of reflectance and transmittance as well as auxiliary measurements of pigment concentrations, thickness and water content for each specimen. For each collected sample, the LOPEX database includes spectral measurements and auxiliary measurements performed at different areas on the leaf surface in order to quantify small local variations.

4.3 Evaluation Data Constraints

The scarcity issue is more prominent with respect to evaluation data. For example, one would assume that there is a large amount of spectral reflectance and transmittance data available for an ubiquitous material such as human skin. Although there have been efforts in order to make such data available in the past (*e.g.*, [121]), there is still a considerable shortage, especially with respect to hyperspectral data. Until recently [31, 89], only a few datasets containing a relatively small number of measurements performed several decades ago (*e.g.*, [62, 61]) were available. The same observations apply to spatial (subsurface scattering and BRDF) data. For example, since Bruls and van der Leun [24] performed their experiments in the 1980's, no significant efforts have been directed to the collection and dissemination of skin subsurface scattering data. The situation is no different for skin BRDF data, with only a few measured datasets being available in the literature (*e.g.*, [79]). It is also important to note that most available datasets are limited to a few illumination and viewing geometries (including LOPEX, which considers only an angle of incidence equal to $8°$).

In order to appropriately compare modeled results with measured data, it is necessary to replicate the actual measurement conditions, such as angle of incidence, collection geometry, spectral resolution (for reflectance and transmittance), wavelength of interest (for scattering measurements) and spectral characteristics of the light source (notably for data obtained using cameras). However, this information is often partially or completely omitted in publications reporting these datasets. Moreover, as mentioned earlier, these publications rarely include specific material characterization data. In many cases, this information is limited to qualitative descriptions. For example, in case of skin data, terms like "Caucasian", "Asian" and "African" are frequently employed despite their poor correlation with a skin specimen's biophysical characteristics [8].

Alternatively, in the absence of data in the literature, one may need to resort to data capture initiatives. In these cases, it is necessary to factor in investments in equipment, space and time. However, although these investments can be substantial, they can bring significant benefits. These include the control over the measurement conditions and a more precise description of the sample materials (specimens). Moreover, by making the collected data available and throughly-documented, one's scope of contributions increases considerably. After all, as recently stated by McNutt [81] "... interpretations come and go, but data are forever."

5 Design Issues

For the sake of completeness and correctness, one would like to take into account all of the structural and optical characteristics of a given material during the model design stage.

However, even if one is able to represent a material in a molecular level, data may not be available to support such a detailed description. Hence, researchers attempt to find an appropriate level of abstraction for the material at hand in order to balance data availability and fidelity issues. No particular modeling design approach is superior for all materials, and regardless of the selected level of abstraction, simplifying assumptions and generalizations are usually employed in the current models due to practical constraints and the inherent complexity of real materials. In this section, we address these issues and their impact on the effectiveness of the existing simulation algorithms.

5.1 Level of Abstraction

There are different ways to represent real materials when it comes to the modeling of their interactions with light. For example, there are models that simulate light transport by geometrically representing each individual material constituent (*e.g.*, the cells found in plant tissues [45]). In theory, this approach would allow for a high degree of fidelity provided that one can obtain the required data to support such detailed material representations. However, in practice, this approach can incur prohibitive computational costs for some applications. For example, in the case of particulate materials like sand or blood, it would be impractical to store all of their constituent elements.

At the other end, there are models that employ the intuitive concept of layers to represent materials whose internal structure has a stratified nature such as human skin. Accordingly, the properties of the material constituents are globally described through mathematical expressions (*e.g.*, using pre-computed functions to represent the bulk scattering of light within a given layer [97]). Although this approach tends to have a lower impact on computational costs, it may lead to a more extensive use of simplifying assumptions and generalizations that can considerably affect the fidelity of the modeled results.

It is also possible to compute the patterns of light propagation and attenuation within a material without resorting to either of these approaches. More specifically, the directional changes can be computed on the fly by taking into account the geometric characteristics of the material constituents without explicitly storing them. This approach was initially employed in the development of a spectral light transport for sand known as SPLITS (*Sp*ectral *Li*ght *T*ransport Model for *S*and) [68]. For materials characterized by a particulate nature, the SPLITS approach can lead to simulation results with a competitive fidelity to cost ratio. For example, besides its use in the predictive modeling of light interactions with sand grains found in terrestrial [10, 69] and extraterrestrial landscapes [11], it has also been employed in the development of a hyperspectral appearance model for human blood, known as CLBlood (*C*ell-Based *L*ight Interaction Model for Human *Blood*) [126].

These distinct representation approaches are not mutually exclusive and, in certain

cases, they can be combined to achieve a higher degree of predictability with respect to material appearance modeling. For example, the hyperspectral skin appearance model, known as HyLIoS (*Hy*perspectral *L*ight *I*mpingement *o*n *S*kin) [29], employs the concept of layers to represent the cutaneous tissues, and the SPLITS approach to simulate light interactions with melanosomes found in some of these tissues. Ultimately, the most suitable approach for a given material will depend on data constraints as well as on the fidelity, performance and usability requirements of the target applications.

5.2 Simplifying Assumptions

A number of simplifying assumptions are usually adopted during the development of material appearance models. In this section, we highlight two of the most pervasive of these assumptions, namely material homogeneity and isotropy.

Although most real materials are characterized by some degree of heterogeneity in their internal structure, most appearance models assume them to be structurally homogeneous. In some cases, this assumption may lead to modeled results that significantly deviate from a material's actual optical behaviour. For example, the optical behaviour of whole blood differs from that of a homogeneous solution with the same concentration of hemoglobin due to the detour and sieve effects outlined earlier (Section 4.1). In addition, motion may also affect the properties of red blood cells, and consequently how light is reflect and transmitted by flowing blood. Experiments described in the literature [23, 76] show that as the shear rate (defined as the velocity gradient in the direction normal to the flow) increases, these cells start to align with their major axis parallel to the flow direction. This change of orientation, in turn, increases light reflection and reduces light transmission. Hence, if one intends to develop a blood appearance model for applications beyond believable image synthesis, these aspects should be accounted for in the model's formulation [126].

Similarly, the effects of melanin on skin color and UV light attenuation are related not only to melanin content, but also to where it is found and how it is dispersed within the cutaneous tissues [1, 87]. Most skin appearance models, however, assume melanin to be uniformly distributed, and do not take into account either the particle nature or the distribution patterns of the melanosomes. As recently demonstrated [29], since these limitations preclude these models from accounting for detour and sieve effects, prominent discrepancies can be observed when their results are compared to measured data, notably in the ultraviolet and blue-end regions of the light spectrum in which the light attenuation within human skin is dominated by melanin.

Most real materials are also anisotropic, *i.e.*, their reflection profile depends on both the polar and the azimuthal angles measured from the material's normal, and used to define the direction of incidence of the incoming light. This macroscopic behaviour is observed

when the material is rotated around its normal (while the illumination and the viewing directions remain unchanged), and the light intensity reflected to the viewer varies. For example, plant leaves characterized by a parallel venation system tend to reflect light more diffusively in a plane perpendicular to the veins than in a plane parallel to them [125]. Most models, however, assume the materials to be isotropic, *i.e.*, the dependence of their reflection profile on the azimuthal angle of light incidence is often omitted in the modeling of their appearance. Although the impact of this assumption may not be critical for some applications, it is worth noting that there has been relevant work on the treatment of anisotropy (*e.g.*, [95]) that could be potentially combined with existing material appearance models.

5.3 Generalizations

Similar to the simplifying assumptions mentioned in the previous section, several material appearance models employ generalizations to bypass data constraints. In this section, we provide two examples of such generalizations.

After performing the measurements of skin subsurface scattering mentioned in Section 4.3, Bruls and van der Leun [24] suggested that their data could be approximated by one of the single particle phase functions tabulated by van de Hulst [117, 118], namely the Henyey-Greenstein phase function (HGPF) [52]. Since then, this function is being employed to approximate the bulk scattering of a wide range of organic and inorganic materials due to its convenient mathematical tractability. The reader interested in a more detailed review of works using this function is referred to a survey article devoted to this topic [14].

It is worth noting that the HGPF was neither based on the mechanistic theory of scattering [60], nor devised to approximate the bulk scattering of these materials [52]. In fact, it has been extensively demonstrated that a generalized use of the HGPF may negatively affect the correctness and predictability of light transport simulations [13, 14, 38, 84]. Clearly, when measured datasets are available, a more reliable option is to use these datasets directly [14, 19]. In the absence of measured scattering data, one may also want to consider the use of simpler functions that can provide approximations with a higher fidelity to cost ratio [30].

Recall that ideally the spatial patterns of light distribution should be represented in terms of BSSRDF (Section 2.3), a function that takes into account the fact that the light incident on material may exit the material at a different location. In order to account for this positional argument, a number of material appearance models (*e.g.*, [35, 63]) use the dipole method. This method and its variations (multipoles) are based on the diffusion theory. This theory, in turn, can be seen as an approximation for equation of radiative transport known as the Boltzmann photon transport equation [57].

Models based on the diffusion theory are amenable to analytic manipulation, place minor constraints on the type of material, and are relative easy to use [98]. However, the

diffusion approximation is applicable only under certain conditions. First, the measurement point needs to be remote from the light source, *i.e.*, at a distance from the surface where the incident light beam has become completely diffuse [55]. Second, the absorption coefficient of the medium needs to be much smaller than its scattering coefficient [34]. In other words, this approximation can be successfully applied only when scattering events are more probable than absorption events. When this condition does not hold, the diffusion theory provides a poor approximation for the photon transport equation [28, 53]. For example, its use is questionable with respect to the simulation of light interactions with human skin tissue in the UV, visible (below 600 nm) and IR (above 1300 nm) spectral domains where attenuation is dominated by absorption [1]. It is worth mentioning that algorithms have been proposed to improve the reliability of diffusion theory approximations (*e.g.*, [33]). However, their effectiveness remains to be verified through direct comparisons with measured data obtained from actual specimens.

6 Evaluation Approaches

As stated earlier, in order to claim that a model is predictive, one has to provide evidence of the fidelity of its results. This makes the evaluation stage essential to assess the correctness of a given model. In this section, we discuss different evaluation approaches, with a particular emphasis on quantitative and qualitative comparisons of modeled results with actual measured data. Although these comparisons are bound by data availability, by isolating the model from the image synthesis pipeline and comparing it with actual measurements, one mitigates the presence of biases in the evaluation process and facilitates the identification of model parameters and algorithms that are amenable to modification and correction. In this section, we also discuss the recurrent issue involving the pursuit of fidelity and its impact on the performance of simulation algorithms, along with strategies employed to maximize the fidelity to cost ratio of computationally intensive models.

6.1 Relative Comparisons

Since computer graphics systems are primarily designed to generate images, it is expected that appearance models be evaluated through a visual inspection of their impact on the these images. Typically, this involves comparisons with images generated using previous models designed for the same material. However, it is necessary to account for the fact that an image synthesis pipeline is composed of different stages, and a computer generated image may be affected by the algorithms and data employed in each of these stages. Considering that a material appearance model is associated with just one of these stages, an evaluation scheme based solely on visual inspection may be misleading. After all, aspects like geometry, texture mapping and tone mapping may bias comparisons of images generated using

distinct image synthesis pipelines.

Hence, to avoid misinterpreting the results of visual comparisons, it is necessary to compare images generated using the same image synthesis pipeline. However, one often has to overcome a major obstacle in this case, namely the unavailability of the code employed in the implementation of the models used in the comparisons. Although one may expect that a given model's algorithms are provided in the article(s) describing it, important details are frequently left to the readers' interpretation, making their implementation another source for the introduction of bias.

For these reasons, it is advisable to evaluate the correctness of an appearance model considering it as a separate unit of the pipeline. In this case, one can use the model's published predictions. In some instances, these are compared with the predictions provided by a reference model. For example, let's consider a case where a reflectance curve provided by model A closely agrees with its counterpart provided by model B. Assuming that model A is faster than model B, one could conclude that the former is technically superior. However, one also has to account for the possibility that both curves can be far from the "real thing", namely the reflectance curve measured for the target material under the same conditions.

In short, although these relative comparisons can provide useful evidence with respect to a model's effectiveness in contributing for the generation of realistic images, they cannot serve as a substitute for comparisons with actual measured data when it comes to the assessment of the correctness of its predictions. These comparisons can be divided into two complementary groups, namely quantitative and qualitative, which are discussed in the following sections.

6.2 Quantitative Comparisons

This approach consists in directly comparing the predictions of a model with measured data. This may require the implementation of virtual devices used to simulate the actual measurement devices (*e.g.*, spectrophotometers used for reflectance and transmittance measurements, and goniophotometers used for BRDF and BTDF measurements [56, 65]). In order to avoid the introduction of undue bias in the comparisons, the formulations of virtual spectrophotometers [20] and virtual goniophotometers [73] should account for the actual measurement (experimental) conditions, which include illumination and viewing geometries.

As also outlined in Section 4.3, detailed descriptions of the specimens' characterization data are rarely provided along with measured datasets. In these cases, one may need to resort to searches for best mach values in the model's parameter space. These searches, however, should be confined to these parameters' actual ranges indicated in the literature. One should also clearly specify the procedures used in the assignment of parameter values. For example, some parameters can be kept fixed (*e.g.*, the refractive indices of material cons-

tituents), while others can be modified based on the specimens description (*e.g.*, the concentration of iron oxides in sand samples).

Sometimes, the visual inspection of plots depicting these comparison may be biased by scaling issues. Accordingly, different metrics, such as root mean square (RMS) errors, are employed to assist in these comparisons. A reference value in this case, may vary depending on the target material and the intended applications. For example, an RMS error less than 0.03 is considered an indication of good spectral reconstruction in remote sensing applications [59]. It is also necessary to consider that even well designed and carefully calibrated devices can yield results from the same specimen that differ from one measurement to the next. These differences, or uncertainties, are caused by variations in the components of the instrument, fluctuations in environmental conditions and changes in the specimen handling procedure [8]. Accordingly, these uncertainties should be also taken into account during the examination of quantitative comparisons.

6.3 Qualitative Comparisons

Qualitative comparisons can be based on visual observations or experimental observations of actual phenomena. As an example of the former case, we can mention the reflectance profiles observed in bifacial plant leaves (*e.g.*, soybean and maple leaves), with one side of a leaf having a distinctly higher reflectance than the other [16]. As an example of the latter case, we can mention the characteristic "omega" shape observed the 400-600 nm region of the spectral reflectance of lightly pigmented skin specimens [71]. Similar examples can be provided with respect to the spatial patterns of light distribution (*e.g.*, the angular dependence of the skin BRDF and the retro-reflection of sand samples).

Qualitative comparisons have three advantages over quantitative ones. First, they are less dependent on data availability issues. Second, they enable a broader assessment of the behaviour of a model under different conditions. Third, they are less susceptible to experimental fluctuations. However, although they may guide the development of a model in the right direction, they are not sufficient to demonstrate its correctness.

Qualitative and quantitative comparisons complement each other in the assessment of a model's predictive capabilities. Furthermore, they are instrumental in the investigation of implementation errors and in the iterative refinement of a model's algorithms. However, it is important to note that, although they provide evidence of the fidelity of a model's predictions, they may not represent a full proof of their correctness, which in most cases is unattainable due to inherent limitations of computer models and the practical constraints affecting the simulations, notably data scarcity.

6.4 Correctness vs. Efficiency

In order to achieve a high level of predictability, some models employ first principles simulation approaches based on detailed representations of a material's morphological characteristics and optical inhomogeneities. These approaches, in turn, apply fundamental principles of physics to a material's microscopic structure in order to build up the bulk behaviour of how it interacts with light [37]. Due to their comprehensive nature, these approaches are bound to incur higher computational costs. The different strategies usually employed to reduce these costs can be loosely divided into two groups: offline and online.

The offline strategies usually involve the pre-computation of variables associated with time consuming algorithms such as those involving random walks [49] within a plant tissue [18] or inside a red blood cell [126]. The values for these variables can then be stored in lookup tables and directly accessed on demand during running time (*e.g.*, [17]). For cases in which the storage of these values requires large multidimensional data structures that can lead to high data access/reconstruction times, numerical techniques like regression analysis, principal component analysis (PCA), and piecewise PCA can be employed and even combined to allow for higher performance rates [21, 69]. The online strategies usually range from simple code optimizations to the use of parallelization techniques (*e.g.*, [72]) and the exploitation of specialized devices (*e.g.*, the graphics processing unit (GPU)) for general purpose computations (*e.g.*, through the Compute Unified Device Architecture (CUDA) platform [88]).

7 Scientific Prospects

Although advances in realistic image synthesis have been directly connected to the development of material appearance models, this line of research is not restricted to computer graphics. In fact, many models developed for rendering applications were built on modeling approaches developed in other fields. Moreover, a number of these models has been evaluated through methodologies that include the comparison of modeled results with actual measured data, an essential requirement in physical and life sciences. As a result, the scope of applications of these models is not restricted to image generation. They can also be used, either in the forward or inverse mode, in a wide range of scientific investigations outside the computer graphics domain. After all, the interest in how light interacts with different materials continues to be a focal point of fundamental scientific research [32, 44], and a catalyst for the development of far-reaching technologies for the improvement of quality of life worldwide [32, 102]. Incidentally, these aspects are being particularly recognized by United Nations this year with the designation of 2015 as the International Year of Light [116].

We remark that in the forward mode, a model is usually employed to generate spectral

radiometric data (*e.g.*, reflectance and transmittance). Comprehensive spectral radiometric datasets can be obtained by varying the input parameters (material characterization data) describing the material's biochemical and biophysical properties. Such datasets can then be used, for example, to develop strategies to predict changes in the concentration and distribution of important material constituents (*e.g.*, melanin in human skin or chlorophyll in plant leaves) triggered by environmental stimuli. In the inverse mode, a model can take as input reflectance and transmittance data measured for the target material, and provide either the quantification of its constituents or information about how it absorbs and scatters light.

In this section, we address aspects related to the use of predictive material appearance models in investigations outside the computer graphics domain. It is important to note that these interdisciplinary applications can only lead to useful scientific insights if the models' predictions can be fully reproduced. For this reason, in this section, we also discuss reproducibility issues.

7.1 Interdisciplinary Applications

As stated earlier, besides contributing to make the image synthesis process more effective across different spectral domains (Figure 5), the development of high fidelity hyperspectral appearance models offers several opportunities for cross-fertilization between computer graphics and other scientific domains. For instance, these models can be used not only to assist scientists through the generation of predictable images of known phenomena, but also to provide a computational platform for the investigation of processes that cannot be fully examined through traditional "wet" experimental procedures. In this section, we present two case studies to illustrate these interdisciplinary applications. We note that these examples are by no means exhaustive, and similar synergistic efforts involving computer models designed for the simulation of other types of biophysical phenomena can be found in the literature (*e.g.*, [100, 111, 120]).

Figura 5. Images generated using the HyLIoS model [29] to illustrate distinct skin appearance features in the ultraviolet (left), visible (center) and infrared (right) spectral domains.

7.1.1 Case 1: Iridal Pigmentation A longstanding issue in biomedical research involves the biophysical factors affecting the color diversity of the human irides and its connection with ocular diseases. Although the pigmentation and morphological characteristics of heavily and moderately pigmented irides have been extensively discussed in the literature, similar studies are scarce for lightly pigmented irides. Epidemiological and statistical studies indicate that individuals with light-colored irides have a higher risk of developing ocular melanoma [106, 108], and a lower probability of surviving the more aggressive metastatic form of this disease [101]. Nevertheless, the interdependence between iris color and the metastatic spread, via blood vessels, of ocular melanomas remains largely unexplained.

Measurements performed on blue irides by Wielgus and Sarna [124] using electron spin resonance spectroscopy detected less melanin in medium blue irides than in light blue irides [124]. It was postulated that this surprising finding could be related to the localization of pigment granules in the iridal layers. Difficulties in performing separate wet measurements on the different iridal layers have precluded the *in situ* verification of this hypothesis, however. Moreover, these experiments are performed under *in vitro* conditions, with the specimens being usually subjected to freezing procedures that can further alter their optical properties.

We have hypothesized that the darker appearance of lightly pigmented irides with low melanin content might result from different distributions of this pigment in the outermost iridal layer, termed stromal layer [15]. Accordingly, we employed an appearance model developed for human iris, known as ILIT (*I*ridal *Li*ght *T*ransport Model) [74], to perform controlled *in silico* experiments in which the distribution of melanin was changed incrementally in the stromal layer of lightly pigmented irides. Through these simulations, we were able to qualitatively reproduce the experimental observations made by Wielgus and Sarna [124]. The results of our simulations indicated that not only the small amount of melanin within the outermost iridal layers, but also its possible predominant presence in the blood irrigated stromal layer should be taken into account in future investigations of biophysical processes responsible for iridal melanoma [15].

7.1.2 Case 2: Relocation of Chloroplasts Monocotyledonous (C4) plants, such as maize (corn) and sugarcane, have a central role in the economy and ecology of our planet. In many regions, the main food sources are based on C4 crops. These crops are also major suppliers of raw materials used in the production of biofuel. Due to their increasing global demand, it becomes essential not only to monitor and analyze the effects of abiotic stress factors, such as limited water and nutrient supplies, on their productivity, but also to determine their ecological impact (*e.g.*, related to their irrigation needs).

The effective monitoring of C4 crops, in turn, requires the detection of spectral changes under *in vivo* conditions, especially with respect to water requirements [112]. However, the spectral data used in studies involving the reduction of foliar water content, particularly

in the more conspicuous moderate range (reduced water content $> 70\%$) [77], is normally obtained under *in vitro* conditions. In these situations, the specimens (leaves) are detached from a living maize plant and usually air dried [26, 113]. Although one might expect that *in vivo* and *in vitro* water reduction procedures would result in similar spectral changes when in both cases the internal arrangement of the foliar tissues is affected by the same amount of water loss, experiments performed by Maracci *et al.* [78] under *in vivo* conditions (by withholding water from the soil) suggest otherwise. More specifically, while the reflectance of maize leaves increases under moderate water content reduction procedures performed under *in vitro* conditions [113], it decreases when maize leaf specimens are subject to the same procedures under *in vivo* conditions [78].

We hypothesized [12] that these apparent conflicting spectral responses are caused by intrinsic differences between *in vivo* and *in vitro* water reduction procedures. More specifically, they may be associated with the intensification of detour effects due to a more homogeneous distribution of chloroplasts triggered by water deficit signals. It is a well-known fact that certain plants have developed adaptive responses, such as chloroplast displacements, which allow them to adjust to different light absorption regimes without changing pigment contents [99, 42]. However, the underlying mechanisms responsible for these responses and their dependence on environmental factors remain incompletely understood [122].

To date, chloroplasts displacements have been associated with light stimulus and mechanical stress. In the former case, the displacements, termed photorelocation movements, can be toward the light (accumulation responses) to maximize photosynthesis or away from the light (avoidance responses) to minimize photodamage. In the case of mechanical stress, when a region of a plant cell of certain species is briefly touched, the chloroplasts around the contact site move away, a response termed mechano-relocation movement [122].

The main challenges to test our hypothesis through traditional "wet" experiments are are twofold. First, the difficulties to perform controlled experiments involving the same specimen under *in vitro* and *in vivo* moderate water reduction procedures. Second, the possibility that the handling of the specimens may result in chloroplasts' mechano-relocation movements that could bias the investigation of putative relocation movements due to water stress.

Hence, in order to further investigate these phenomena, we used an appearance model for plant leaves, known as ABM-U (*A*lgorithmic *B*DF *M*odel for *U*nifacial Plant Leaves) [9], to qualitatively reproduce the spectral responses obtained in the *in vitro* and *in vivo* experiments performed by Thomas *et al.* [113] and Marraci *et al.* [78], respectively. This model incorporates a bound for angular light (ray) deviations caused by the heterogeneous distribution of chloroplasts. By removing this bound for the *in vivo* water stressed specimen (while keeping all other parameters fixed for both specimens), we were able to demonstrate that our hypothesis is plausible [12]. Although our findings need to be confirmed by more comprehensive investigations involving biochemical processes that might be responsible by this

putative rearrangement of chloroplasts, they provide new insights on the adaptive responses of monocotyledonous C4 plants to unfavourable environmental conditions, and suggest the possibility of an unforeseen third type of chloroplast displacement mechanism triggered by water stress [12].

7.2 Reproducibility

It is widely recognized that reproducibility is the ultimate standard by which scientific contributions should be evaluated. Through replication, independent researchers can address a scientific hypothesis and build up evidence to support or refute it [93]. This principle, however, is often overlooked in several areas, including material appearance modeling.

The full reproduction of a model's predictions calls for the disclosure of data and computer software. The former involves not only the report of all values assigned for the model's parameters used in the simulations, but also the bibliographic or experimental references for these values so that researchers can directly assess their validity. The later may include source and/or object code.

As mentioned earlier (Section 6.1), even though one should expect that all relevant formulation details of a model are provided in the publication(s) describing it, for different reasons this may not occur in practice. In these cases, the implementation of a model by an independent researcher may deviate from its original implementation. Hence, an attempt to replicate published predictions of a model may be biased by implementation issues.

Ideally, the source code for a model should be released along with its publication. However, different issues, such as intellectual property concerns and code documentation overhead [83], usually prevent this from happening. Moreover, even making the source code available may not be enough since the relative complexity of material appearance models, especially for users with limited programming experience, usually prevents their use and the assessment of their effectiveness beyond the boundaries of the research groups responsible for developing and maintaining these models. Incidentally, this problem is also observed in other areas of research [64, 82], and it has triggered efforts for the development of easy-to-use simulation tools by the software industry [105].

Alternatively, model developers can consider the simple release of their model's object code or its deployment using interfaces that can allow users to run it remotely. For example, we have introduced the Natural Phenomena Simulation Group Distributed (NPSGD) framework [7, 85] for the online running of material appearance models developed by our research group. NPSGD was designed to make these models broadly useful to students and researchers interested in the optical properties of natural materials and their spectral responses to environmental changes. It is worth noting that similar initiatives have been implemented in other fields (*e.g.*, [36, 58, 123]).

Clearly, such model deployment initiatives incur significant computational resources and time investments. However, besides providing a sound compromise between code availability and due diligence in the dissemination of research results, they can also lead to other tangible benefits. These include timely opportunities for code improvements. For example, one of our models, BioSpec (*Bio*physically-Based *Spec*tral Model for Human Skin) [71], was reimplemented by different programmers. This allowed us to filter out bugs and improve model running performance by using more efficient software and hardware features [5]. Moreover, these deployment initiatives enhance the ability of the scientific community at large to engage in the research work behind these models.

8 Conclusion

The development of material appearance models capable of providing predictive results within and outside the visible spectral domain can open new avenues of research in computer graphics and related areas. It can also lead to relevant advances in the life and physical sciences. However, besides the acquisition of a comprehensive understanding about the target material from a biophysical perspective, it also requires substantial professional and personal investments to overcome technical and political barriers. While the former are associated with objective problems such as data scarcity, terminology inconsistencies and unsound generalizations, the later are related to subjective, albeit no less significant, issues that may involve, for example, different interpretations of the quality and merits of one's work by paper and grant reviewing committees. Is it worth the effort? It depends on how useful one aims for his/her work to be.

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