Predictive Modeling of Material Appearance: From the Drawing Board to Interdisciplinary Applications

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Abstract

This tutorial addresses one of the fundamental and timely topics of computer graphics research, namely the predictive modeling of material appearance. Although this topic is deeply rooted in traditional areas like rendering and natural phenomena simulation, this tutorial is not limited to cover contents connected to these areas. It also closely looks into the scientific methodology employed in the development of predictive models of light and matter interactions. Given the widespread use of this methodology to find modeling solutions for problems within and outside computer graphics, its discussion from a "behind the scenes" perspective aims to underscore practical and far-reaching aspects of interdisciplinary research that are often overlooked in related publications. More specifically, this tutorial unveils constraints and pitfalls found in each of the key stages of the model development process, namely data collection, design and evaluation, and brings forward alternatives to tackle them effectively. Furthermore, besides being a central component of realistic image synthesis frameworks, predictive material appearance models have a scope of applications that can be extended far beyond the generation of believable images. For instance, they can be employed to accelerate the hypothesis generation and validation cycles of research across a wide range of fields, from biology and medicine to photonics and remote sensing, among others. These models can also be used to generate comprehensive in silico (computational) datasets to support the translation of knowledge advances in those fields to real-world applications (e.g., the noninvasive screening of medical conditions and the remote detection of environmental hazards). In fact, a number of them are already being used in physical and life sciences, notably to support investigations seeking to strengthen the current understanding about material appearance changes prompted by mechanisms which cannot be fully studied using standard "wet" experimental procedures. Accordingly, such interdisciplinary research initiatives are also discussed in this tutorial through selected case studies involving the use of predictive material appearance models to elucidate challenging scientific questions.

Keywords: material appearance modeling, natural phenomena simulation, rendering, realistic image synthesis, scientific methodology and interdisciplinary applications.

Categories and Subject Descriptors (according to ACM CCS): I.3.7 [Computer Graphics]: Three-Dimensional Graphics and Realism—I.3.8 [Computer Graphics]: Applications—

1. Outline

This tutorial is composed of six main sections. The topics covered in each of these sections are concisely described as follows:

- Section 1. Provides the required background and terminology to be employed throughout the tutorial. We start with a brief description of the main processes involved in the interactions of light with matter and a review of relevant optics concepts. We then concisely present the group of radiometric measurements (*e.g.*, reflectance, transmittance and scattering functions [NRH*92]) that characterize the spectral and spatial distribution of light propagated by a given material and determine its appearance attributes (*e.g.*, colour, glossiness, translucency) [HH87].
- Section 2. To establish whether a model can be considered predictive, one has to assess the fidelity of its predictions, *i.e.*, the degree to which they can reproduce the state and behaviour of a real world material in a measurable manner [Gro99]. Accordingly, we examine these pivotal concepts and the trade-offs associated with their adoption in the design of models to be incorporated not only into realistic image synthesis frameworks, but also into *in silico* experimental platforms for physical and life sciences research. We also provide an overview of the main design strategies and simulation approaches employed in the development of predictive material appearance models.
- Section 3. It has been long recognized [War92] that a carefully designed model is of little use without data. In the case of

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predictive material appearance models, one needs material characterization data (*e.g.*, thickness and pigment content) to be used as input, fundamental biophysical data (*e.g.*, specific absorption coefficients for the pigments) to support the light transport simulations, and evaluation data (*e.g.*, hyperspectral reflectance datasets) to assess the fidelity of the modeled quantities. Ideally, the characterization and evaluation data should correspond to the same material sample. However, this is rarely the case, with measured datasets available in the literature commonly lacking a detailed description of the material samples used in the measurements. Fundamental data for materials in their pure form, such as natural pigments, can pose significant challenges as well. For instance, their absorption spectra are often obtained either through inversion procedures, which may be biased by the inaccuracies of the inverted model, or may not take into account *in vivo* and *in vitro* discrepancies. In this section, we discuss these and other issues related to data availability and quality, and how they affect the models' predictive capabilities. We also highlight alternatives to mitigate these issues.

- Section 4. For the sake of completeness and correctness, one may want 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 target material in order to balance data availability, fidelity issues and application requirements. No particular modeling approach is superior in all cases, and regardless of the selected level of abstraction, simplifying assumptions and generalizations are usually incorporated into the models' formulation 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 simulation algorithms employed by these models.

- Section 5. The evaluation stage is essential not only to determine the predictive capabilities of a given model, but to iteratively refine its design. In this section, we discuss different evaluation approaches, with a particular emphasis to quantitative and qualitative comparisons of modeled results with actual measured data and/or experimental observations. Although this approach is bound by data availability, it 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 trade-off involving the pursuit of fidelity and its impact on the performance of simulation algorithms, along with strategies employed to maximize the fidelity/cost ratio of computationally intensive models.

- Section 6. The development of predictive material appearance models offers several opportunities for synergistic collaborations between computer graphics and other scientific domains. We remark that predictive models can provide a robust computational platform for the *in silico* investigation of phenomena that cannot be fully examined through traditional laboratory procedures. Eventually, these investigations can also lead to significant model enhancements. In this final section, we employ case studies to examine these positive feedback loops. We also discuss the importance of reproducibility, the cornerstone of scientific advances, and address technical and subjective barriers that one may need to overcome in order to establish fruitful interdisciplinary collaborations.

2. Syllabus

The tutorial syllabus and the time allocated for each of its sections are provided below:

- Introduction (10 min)
- Section 1: Biophysical Background (25 min)
  - Light and Matter Interactions
  - Optics Concepts
  - Measurement of Appearance
- Section 2: Drawing Board (20 min)
  - Predictability Guidelines
  - Framework Choices
- Section 3: Data Availability and Quality (35 min)
  - Biophysical Data Constraints
  - Characterization Data Constraints
  - Evaluation Data Constraints

  Break

- Section 4: Design Issues (30 min)
  - Level of Abstraction
  - Simplifying Assumptions
  - Generalizations and Pitfalls
  - Iterative Refinement
  - Algorithmic Evolution
- Section 5: Evaluation Approaches (20 min)
  - Relative Comparisons
  - Qualitative Comparisons
  - Quantitative Comparisons
  - Correctness vs. Efficiency
- Section 6: Interdisciplinary Applications (35 min)
  - Scope of Applications
  - Case Studies
  - Reproducibility
- Conclusion (5 min)

3. Intended Audience and Background

The intended audience includes graduate students, practitioners and researchers, from both academia and industry. As mentioned earlier, although the tutorial's main topic is connected to traditional areas of computer graphics, such as rendering and natural phenomena simulation, its contents and delivered insights are likely to be of interest to attendees from other areas. Accordingly, a concise background section is included in the proposed schedule to ensure that attendees from different areas can get the most of the tutorial. Experience with specific simulation techniques, such as those based on the use of Monte Carlo methods [BK10], would be helpful, but it is not required.

4. Presenter's Brief Resume

Gladimir Baranoski is a professor of computer science at the University of Waterloo (Canada), where he has established the Natural Phenomena Simulation Group (NPSG). His current research interests include material appearance modeling, natural phenomena simulation and biophysically-based rendering. The results of his interdisciplinary research on the predictive modeling of light and matter interactions have been made available to the scientific community through the publication of articles in journals and conference proceedings in computer graphics and related fields such as biomedical optics and remote sensing. He has also co-authored books and book chapters as well as organized a number of tutorial/course presentations for computer graphics conferences (*e.g.*, CGI (2000), SIBGRAPI (2002, 2004 and 2015), EUROGRAPHICS (2001, 2002 and 2005), SIGGRAPH (2002 and 2003), SIGGRAPH Asia (2008 and 2009)), and remote sensing events (*e.g.*, IEEE International Geoscience and Remote Sensing Symposium - IGARSS (2008, 2009, 2020 and 2023)), on topics related to the main theme of this proposal.

5. Tutorial History

This tutorial builds on the experience of delivering similar presentations for the aforementioned events, and on the lessons learned during the development of a number of predictive models of light interactions with organic materials (*e.g.*, plants [BR97, BR01, BR04, Bar06] and human tissues like skin [KB04, BK10, BCK14, CBKM15], iris [LB06, KBC*17], blood [YBK*12]) and inorganic materials (*e.g.*, sand [KB07, KB10] and snow [VBK21, VB24]). It also aggregates insights obtained from employing those models in interdisciplinary research initiatives spanning a myriad of topics, such as the investigation of environmentally-elicited material appearances changes (*e.g.*, [BKCY12, KBC*13, CB19]), the noninvasive and remote assessment of material properties (*e.g.*, [BL07, BKCM14, BKCM15, BC17, BKVI19, BIK*21, BI23, vB18, vB19, VB21, BV24]), and the screening of medical conditions (*e.g.*, [BCK*12, CSB13, BDC15, BLC17, AB18]), just to name a few.

A similar version of this tutorial has been presented in the SIBGRAPI 2015 [Bar15]. Since then, the interest and the research on its main topic continue to evolve along with its scientific ramifications. Its contents have been updated to reflect these aspects and to enable its delivery to a broader audience. Recently, its enhanced version was presented in the IGARSS 2023, the premier event in remote sensing, held in Pasadena, CA, USA, in July 2023.

For this EUROGRAPHICS 2024 offering, the tutorial organization and contents were further refined to incorporate new insights derived from recent developments in related areas. Moreover, this version will emphasize aspects related to computer graphics applications, while the version presented at IGARSS 2023 highlighted aspects associated with remote sensing applications.

6. Deliverables

We remark that this tutorial aims to address practical issues that may arise during the development of predictive material appearance models. The discussion of these issues is illustrated by examples obtained from models whose published descriptions (publications) and website interfaces can be accessed online (*http://www.npsg.uwaterloo.ca/index.php*) along with related images (*e.g.*, Fig. 1) and videos respectively presented and cited in the accompanying slides.

Figure 1: *Images illustrating the use of predictive material appearance models in biophysically-based rendering.*

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