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

Gladimir V. G. Baranoski

Natural Phenomena Simulation Group
D.R. Cheriton School of Computer Science
University of Waterloo, Canada

EUROGRAPHICS 2024 – Limassol, Cyprus

Schedule

- ❑ Introduction
- ❑ Biophysical Background
- ❑ Drawing Board
- ❑ Data Availability and Quality

Break

- ❑ Design Issues
- ❑ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

Introduction

- Scope
- Goals
- Materials of Interest
- Final Destination

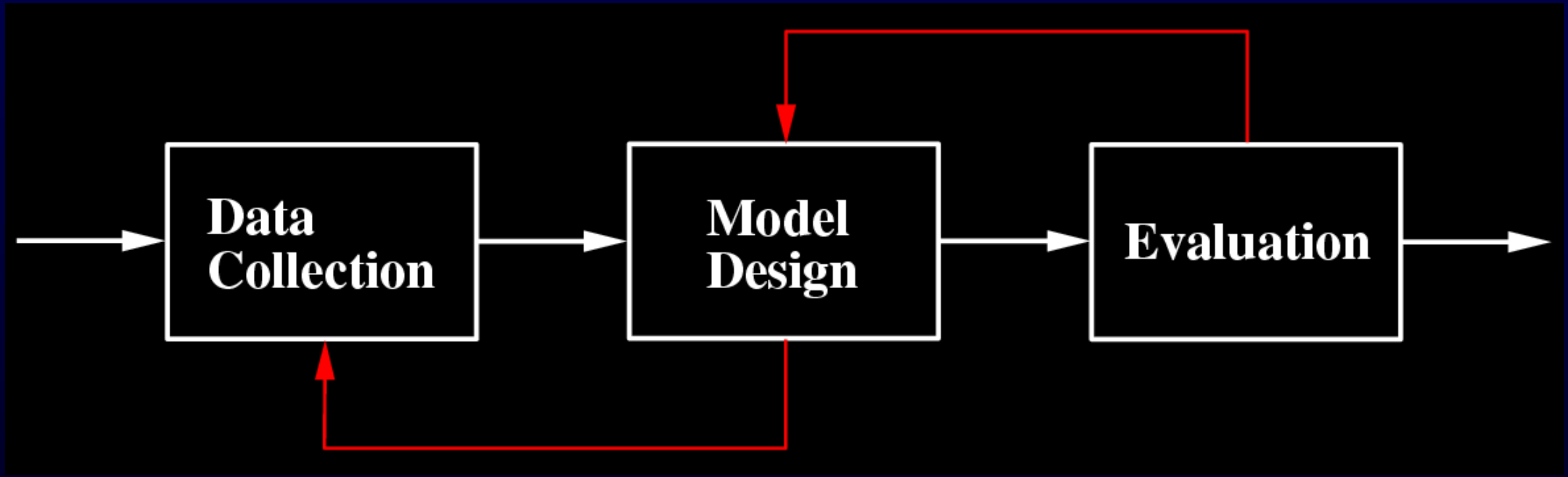
- Scope: predictive modeling of light and matter interactions

➢ Materials of interest: organic …

… and inorganic

➢ Goals

- To discuss practical challenges that need to be addressed during the model development process

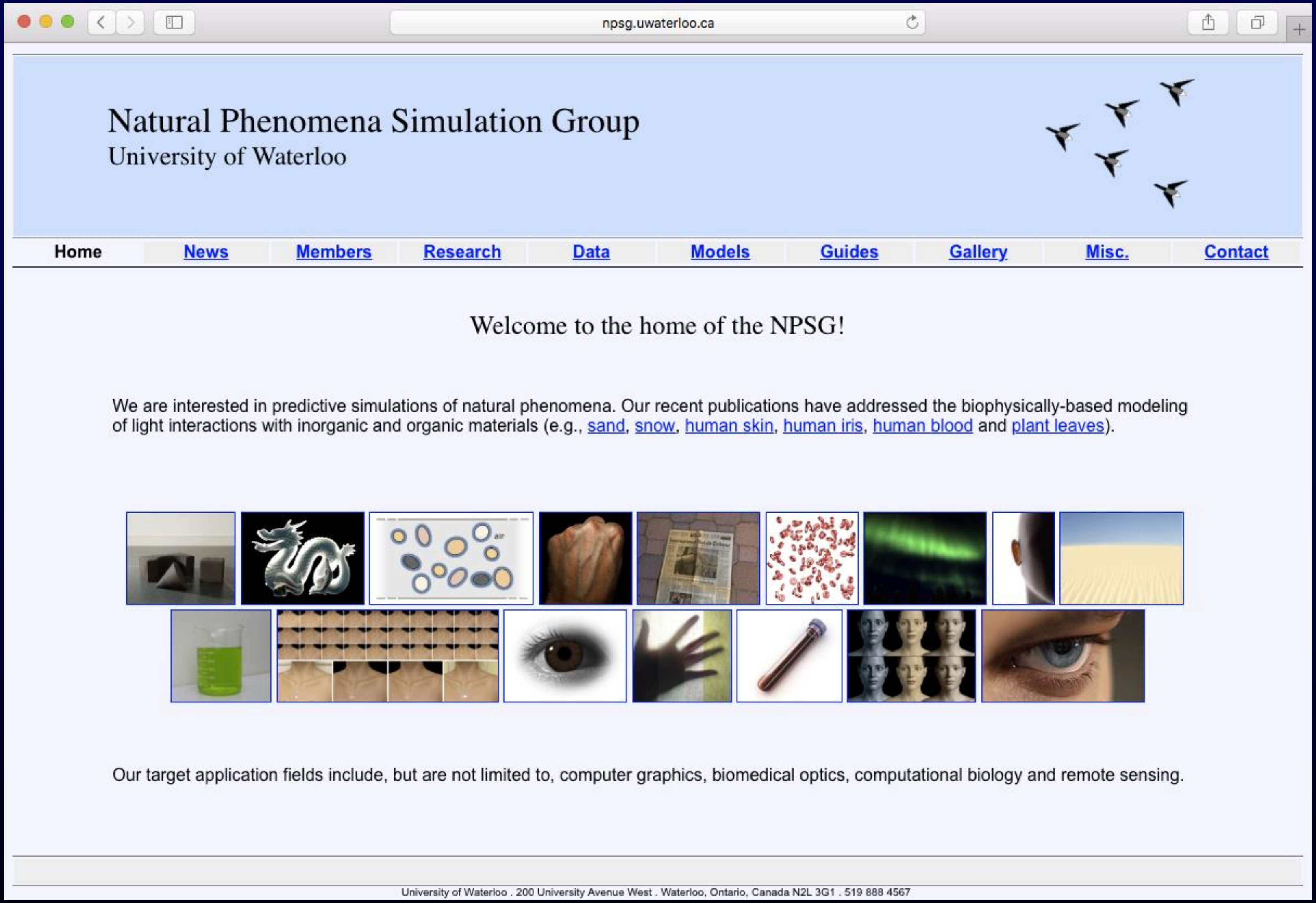


- To share the “lessons” learned from our past and ongoing experiences in this area

- Among those experiences, we highlight the development of predictive light transport models for different materials

  - Snow: SPLITSnow (*Remote Sensing of Environment (RSE)* 2021)
  - Human skin: BioSpec (*EG* 2004) and HyLIoS (*ACM TOG* 2015)
  - Human blood: CLBlood (*EG* 2012)
  - Sand: SPLITS (*Optics Express* 2007)
  - Human iris: ILIT (*EG* 2006)
  - Plant leaves: ABM (*EG* 1997), ABM-B and ABM-U (*RSE* 2006)

- Supporting materials can be found at:



http://www.npsg.uwaterloo.ca

➢ Final destination: interdisciplinary applications

Schedule

- ✓ Introduction
- ❑ Biophysical Background
- ❑ Drawing Board
- ❑ Data Availability and Quality

Break

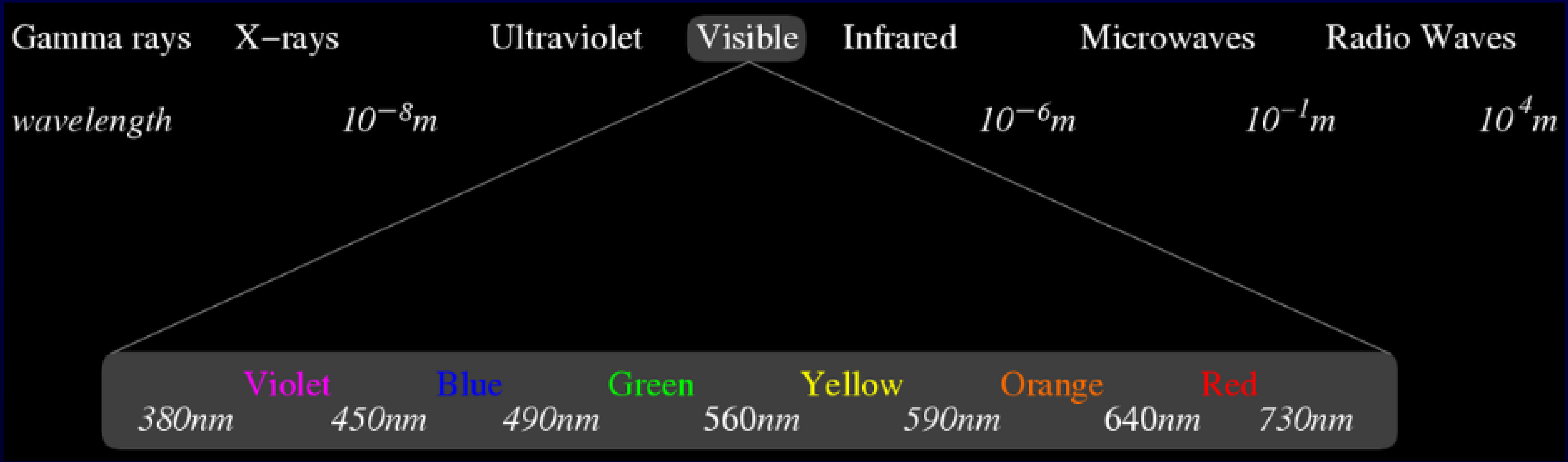
- ❑ Design Issues
- ❑ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

Biophysical Background

- Light Interactions with Matter
- Optics Concepts
- Measurement of Appearance

Light Interactions with Matter

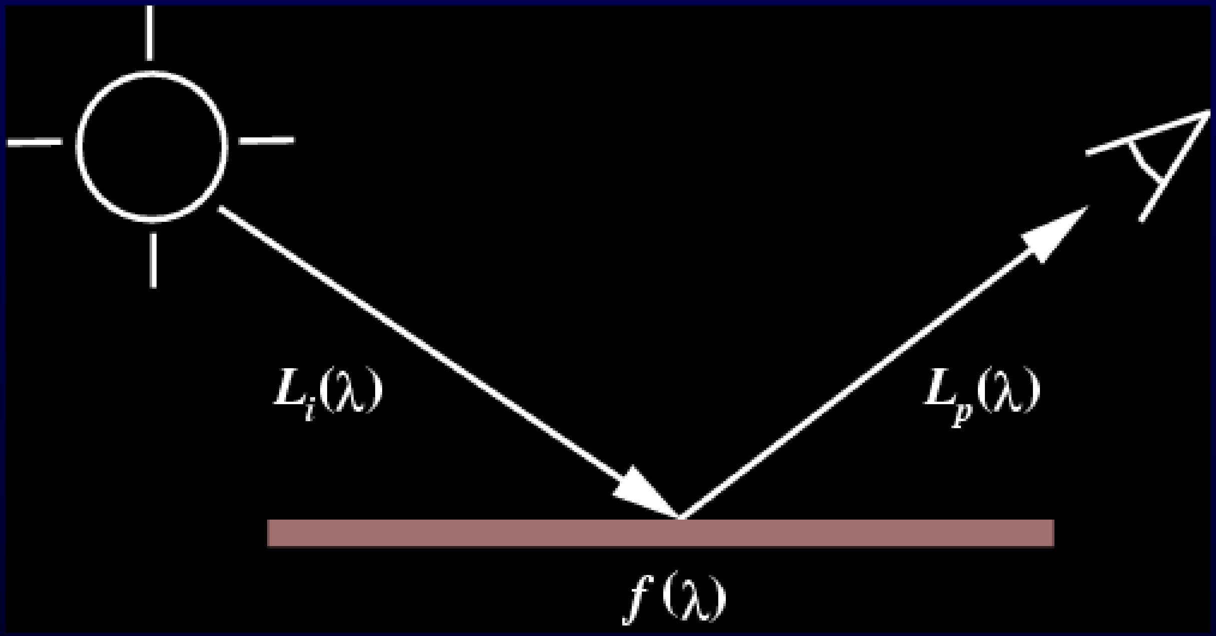
➢ Light as electromagnetic radiation (form of energy)



➢ Dual nature of light

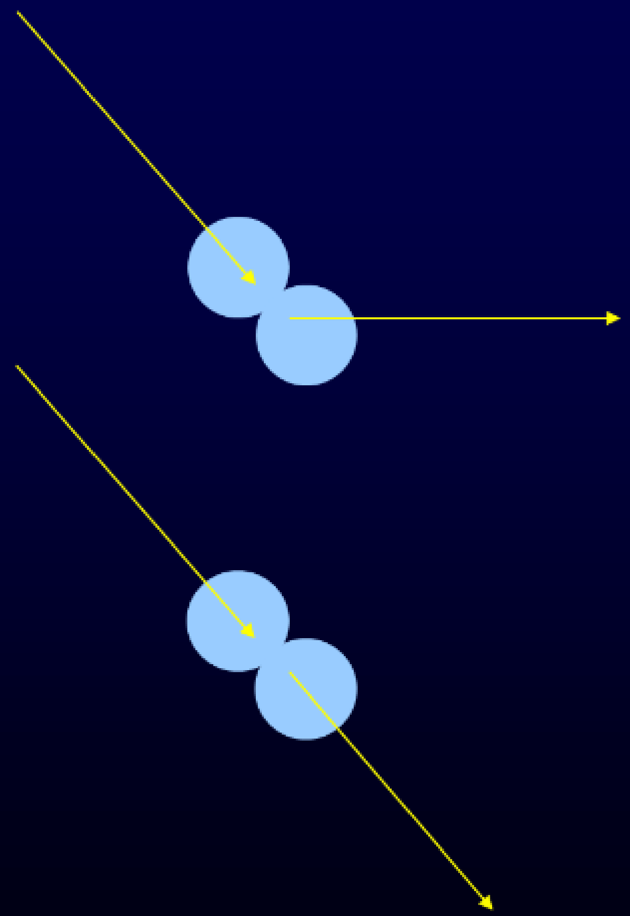
- Wave and particle (photon)

➢ Light and matter interaction phenomena



- Scattering

  - Deflection of photons through collisions with material particles



- Main types found in nature:
  - Rayleigh scattering
  - Mie scattering
  - Reflective-refractive (geometrical optics)

- Remark: in reality, these are complex phenomena

- If we want to know more about these phenomena, then we should take a look at:

QED – The Strange Theory of Light and Matter
R.P. Feynman (1985)

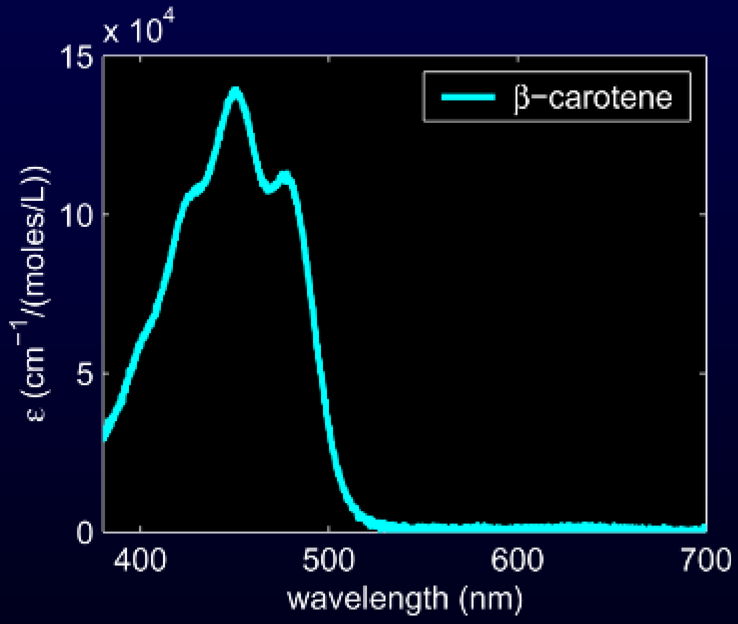
- Absorption

  - Once light is transmitted into a medium, it may be absorbed due to the presence of pigments (chromophores) or dyes

  - Absorption is affected by:
    - ❖ the distribution of the absorptive elements (absorbers)
    - ❖ the concentration of the absorbers
    - ❖ the specific absorption coefficient (s.a.c.) of the absorbers

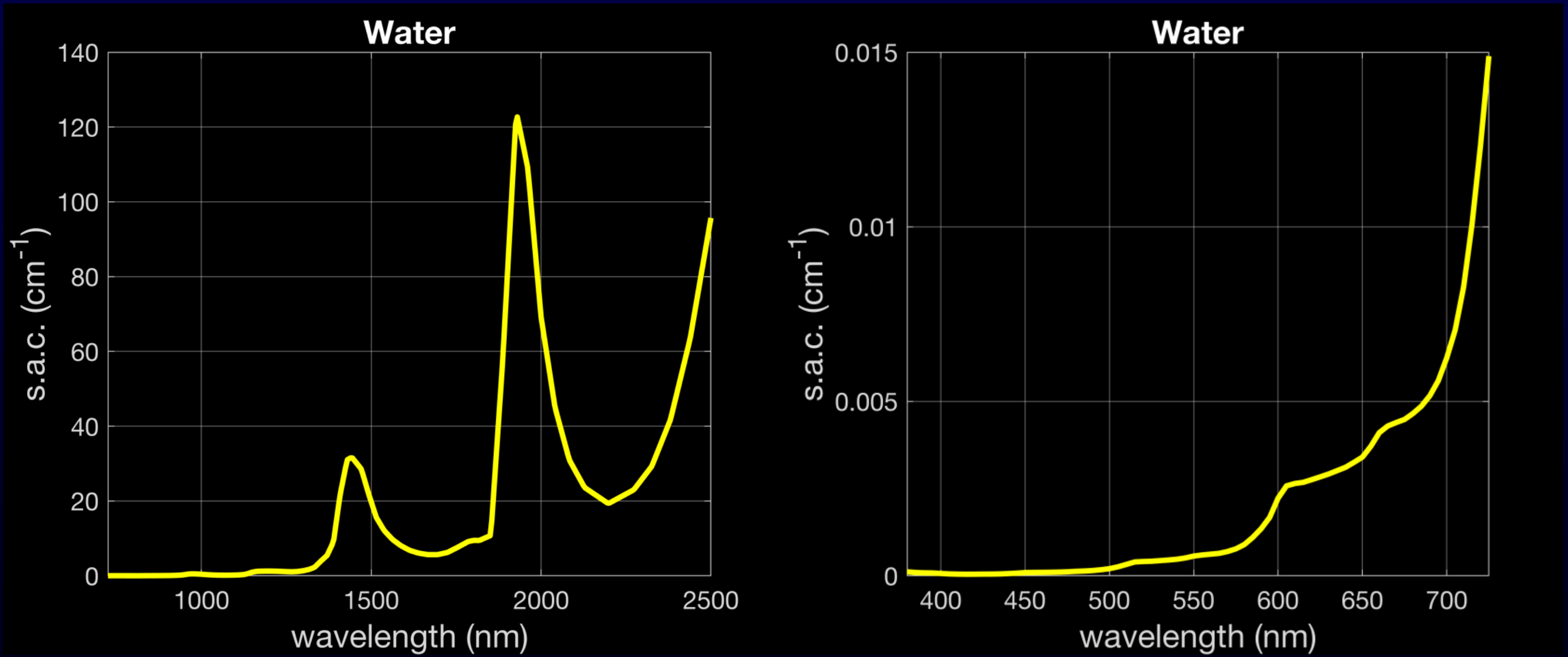
- Remark:

  - The <u>specific absorption coefficient</u> (s.a.c.) of an organic pigment can be obtained by dividing its molar extinction coefficient by its molecular weight



- The s.a.c. of an inorganic material can be computed from its extinction coefficient (k) by employing the following formula:

$$\zeta(\lambda) = \frac{k(\lambda)4\pi}{\lambda}$$



Optics Concepts

- **Attenuation coefficient:** corresponds to the sum of the scattering coefficient and absorption coefficient

- **Albedo:** represents the ratio of the scattering coefficient to the attenuation coefficient

$$\gamma(\lambda) = \frac{\mu_s(\lambda)}{\mu_s(\lambda) + \mu_a(\lambda)} = \frac{\mu_s(\lambda)}{\mu(\lambda)}$$

where:

$$\begin{aligned} \mu_s &= \text{scattering coefficient}, \\ \mu_a &= \text{absorption coefficient}, \\ \mu &= \text{attenuation coefficient}. \end{aligned}$$

- Remarks

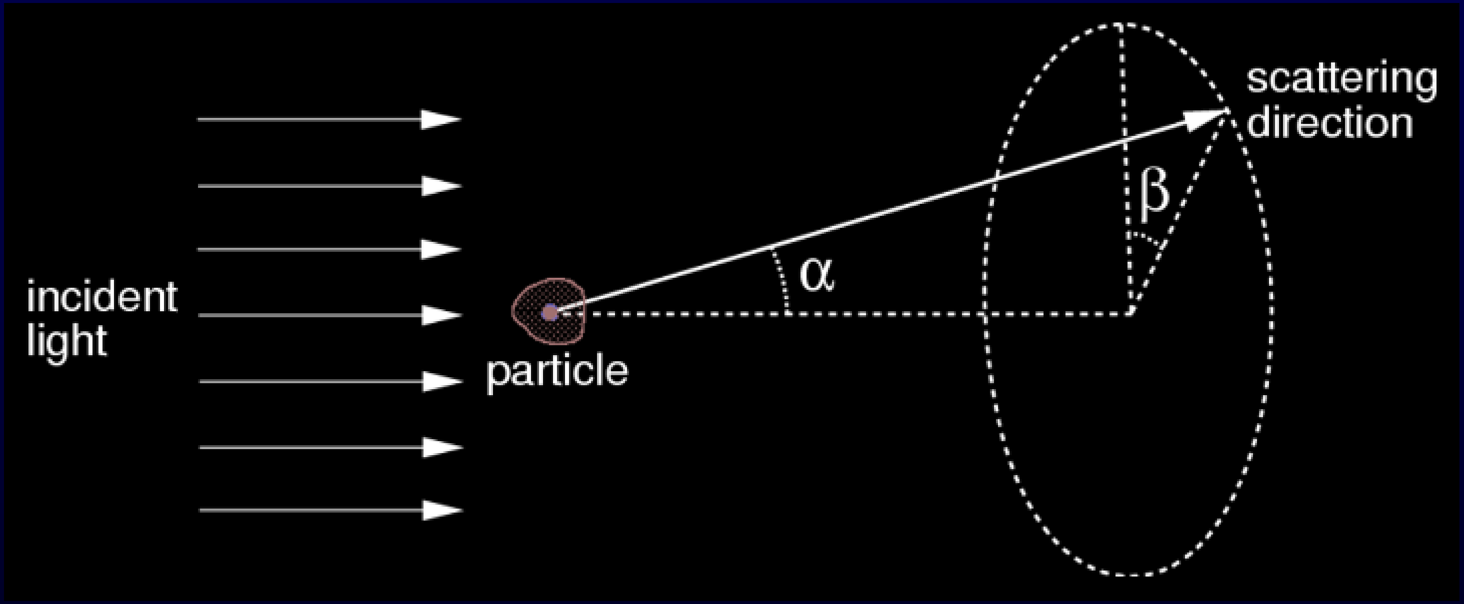
  - In some areas, these coefficients are usually used to describe the light attenuation behaviour of a whole material/tissue

  - Watch out for:

    - the introduction of undue inaccuracies

    - the scarcity of directly measured data

- **Phase function:** represents the directional scattering of the light incident onto a particle



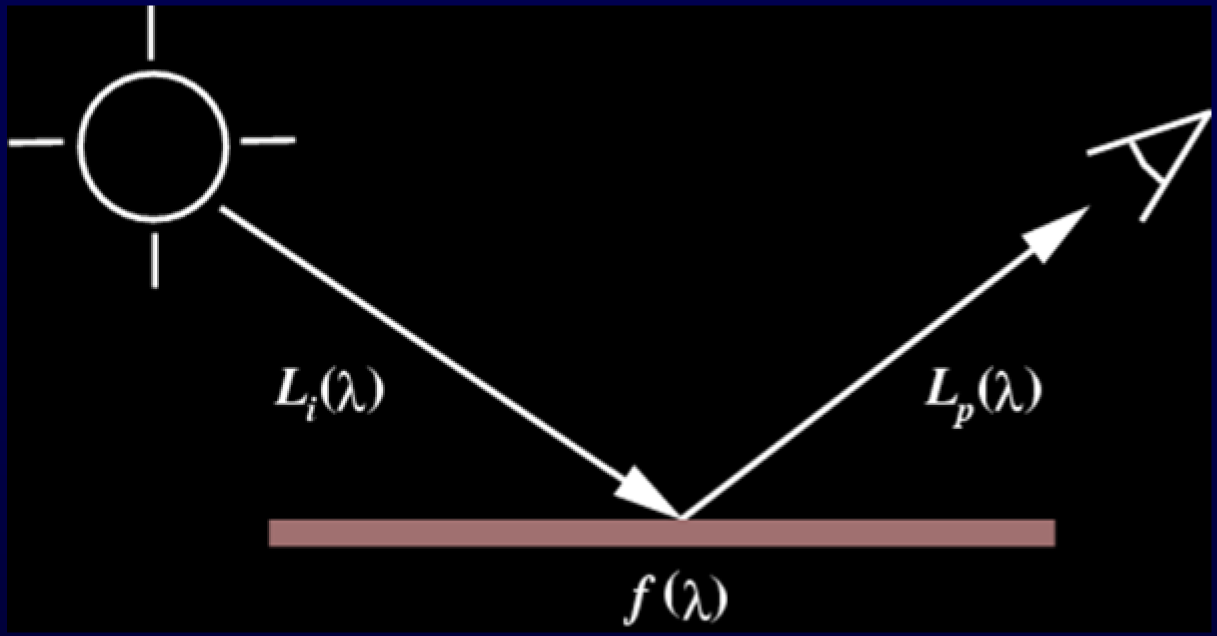
Measurement of Appearance

"Group of measurements that characterizes both the color and the surface finish of an object."

Hunter and Harold (1987)
The Measurement of Appearance

- Spectral light distribution
  - How does it affect appearance?
    - Hue (color), saturation and lightness

- Spatial light distribution
  - How does it affect appearance?
    - Glossiness, translucency, transparency etc…



$L_i(\lambda)$
$L_p(\lambda)$
$f(\lambda)$

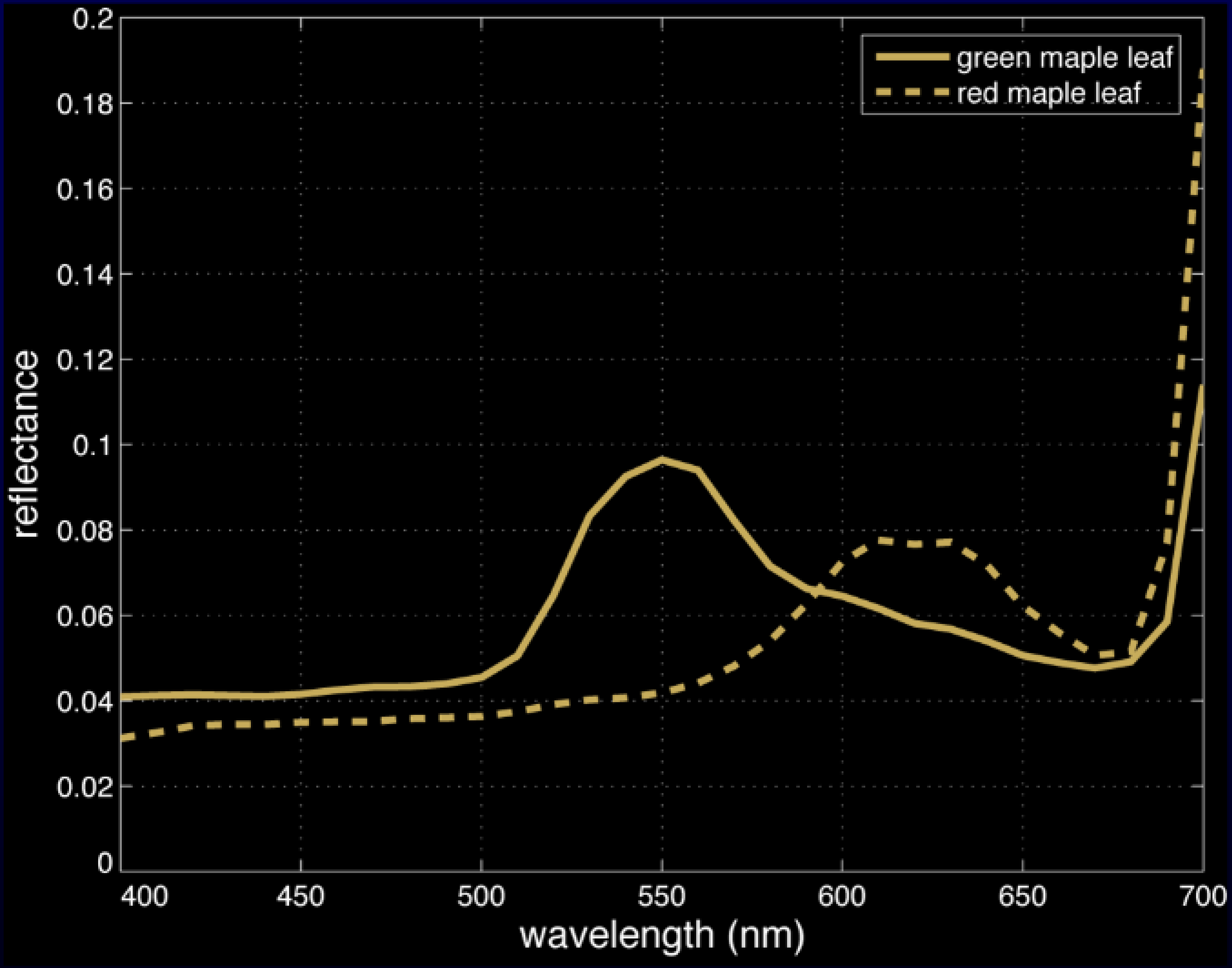
➢ Measuring spectral light distribution

- Spectral reflectance:
  - ratio of the reflected to incident radiant flux (power) for a given wavelength

$$\rho(\lambda) = \frac{\Phi_r(\lambda)}{\Phi_i(\lambda)}$$

  - always between 0 and 1 (conservation of energy)
  - dimensionless

Spectral Reflectance of Green and Maple Leaves



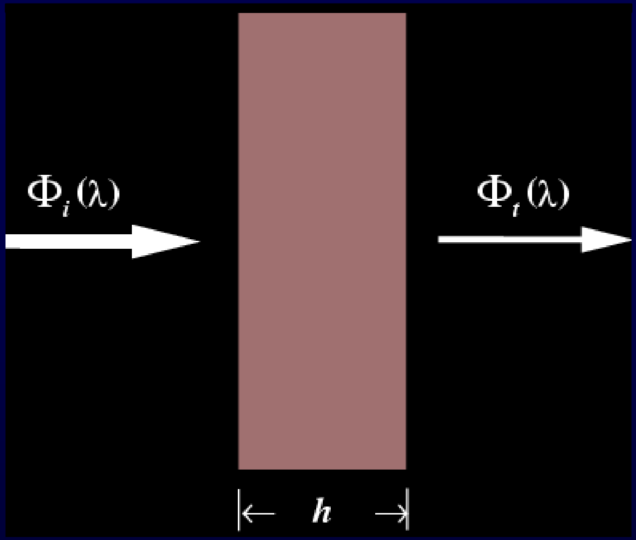
- Spectral transmittance:
  - ratio of the transmitted to the incident radiant flux for a given wavelength

$$\tau(\lambda) = \frac{\Phi_t(\lambda)}{\Phi_i(\lambda)}$$

  - always between 0 and 1 (energy conservation)
  - dimensionless
  - reflections at the surface as well as absorption within the material operate to reduce the transmittance

- Lambert's law of absorption (Bouguer's law)

$$\tau(\lambda) = \frac{\Phi_t(\lambda)}{\Phi_i(\lambda)} = e^{-\zeta(\lambda)\ h}$$



where:

$\zeta(\lambda)$ = specific absorption coefficient of the medium at λ,

h = thickness of the medium,

e = Euler's number.

- Beer's law: for a dye solution, the loss due to absorption is proportional to the dye's concentration (c)

- Combining these laws: $\tau(\lambda) = e^{-\zeta(\lambda)\ c\ h}$

- Spectral absorptance:
  - ratio of the absorbed to the incident radiant flux for a given wavelength

$$\mathcal{A}(\lambda) = \frac{\Phi_a(\lambda)}{\Phi_i(\lambda)}$$

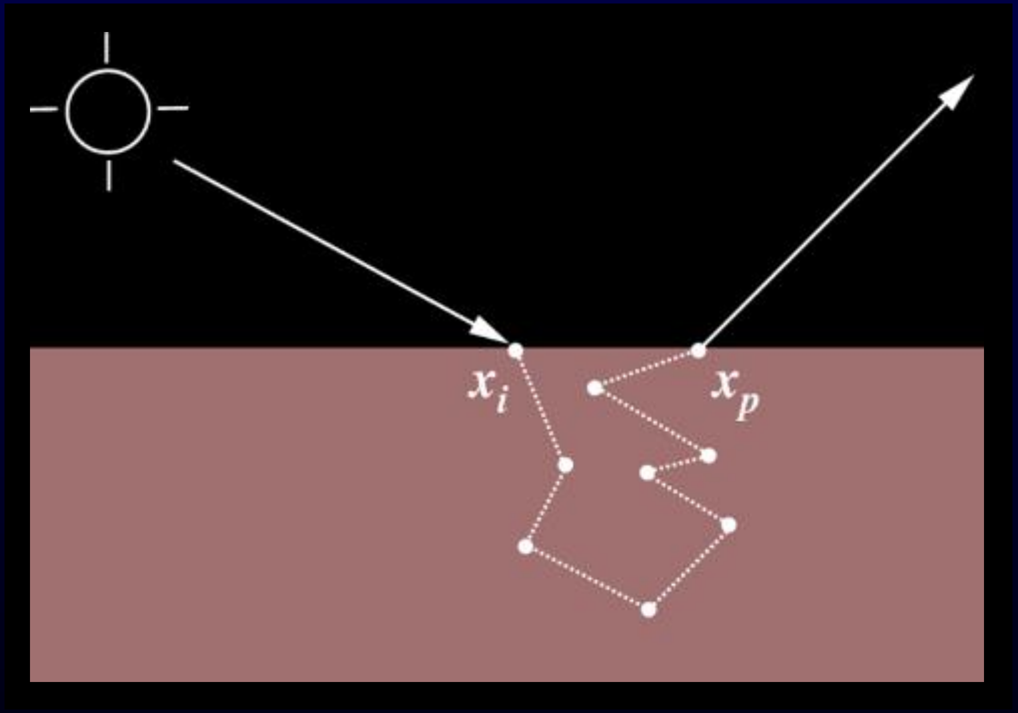
  - dimensionless

- Due to energy conservation, the following relationship holds:

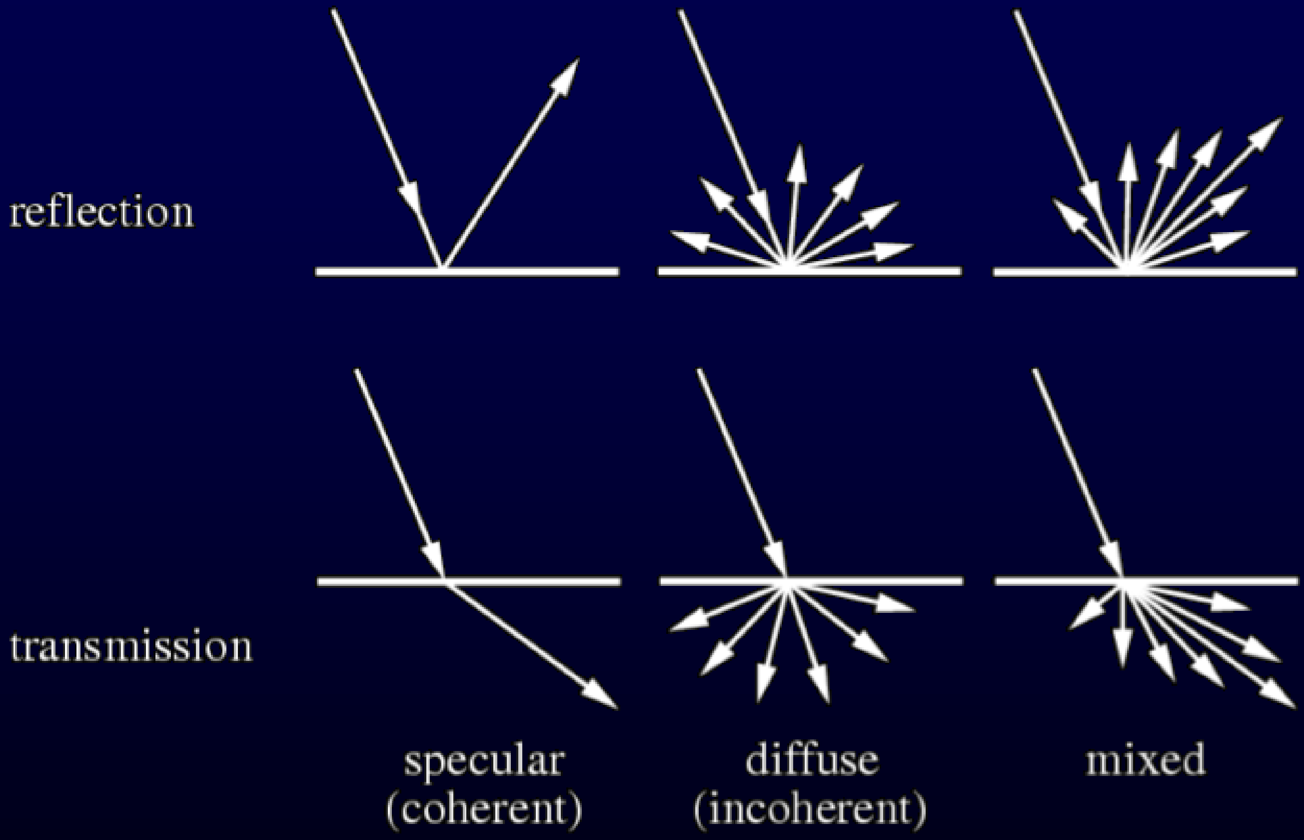
$$\rho(\lambda) + \tau(\lambda) + \mathcal{A}(\lambda) = 1$$

➢ Measuring spatial light distribution

- Bidirectional scattering-surface distribution function (BSSDF): positional dependence



• Bidirectional scattering distribution function (BSDF or BDF): positional dependence is assumed to be negligible



- Bidirectional scattering distribution function (BSDF or BDF): positional dependence is assumed to be negligible
    - Bidirectional Reflectance Distribution Function (BRDF)
    - Bidirectional Transmittance Distribution Function (BTDF)

- BSDF (in sr^{-1}) is given by:

$$f(\psi_i, \psi, \lambda) = \frac{dL(\psi, \lambda)}{L_i(\psi_i, \lambda)\, d\vec{\omega}_i\, cos\theta_i}$$

where:

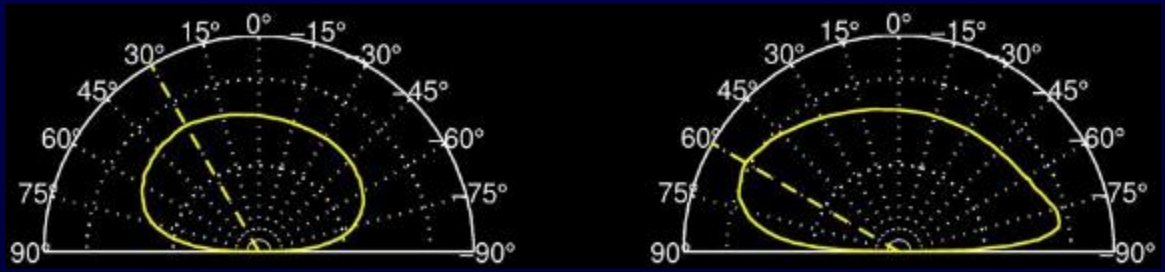
$dL(\psi, \lambda)$ = radiance propagated in a direction ψ,

$L_i(\psi_i, \lambda)$ = incident radiance in a direction ψ_i,

θ_i = angle between the surface normal and ψ_i,

$d\vec{\omega}_i$ = differential solid angle at which L_i arrives at the surface.

Examples of BRDF Profiles of Sand



Schedule

- ✓ Introduction
- ✓ Biophysical Background
- ❑ Drawing Board
- ❑ Data Availability and Quality

Break

- ❑ Design Issues
- ❑ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

Drawing Board

- Predictability Guidelines
- Framework Choices

Predictability Guidelines

➢ What does predictability entail?

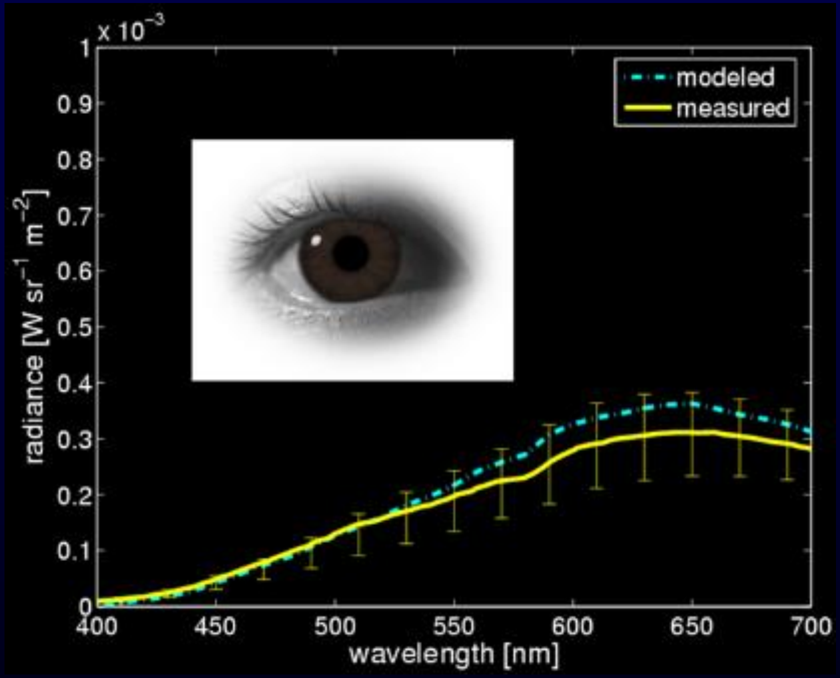
- Fidelity

“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.”

D. Gross (1999)
Report from the Fidelity Implementation Study Group

Predictability Guidelines

- What does predictability entail?
  - Fidelity

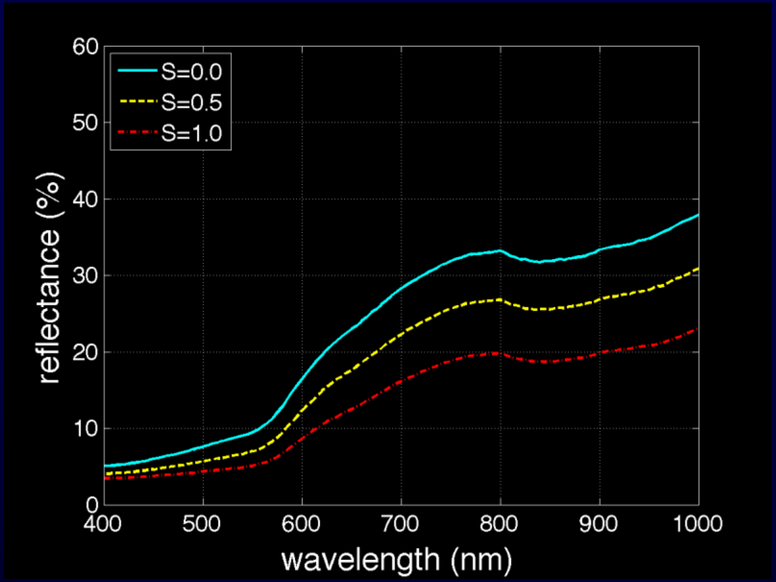


(Measured data provided by F. Imai 2000)

- Models controlled by (bio)physically meaningful parameters

Example:

variations in the degree of water saturation (S) of sand

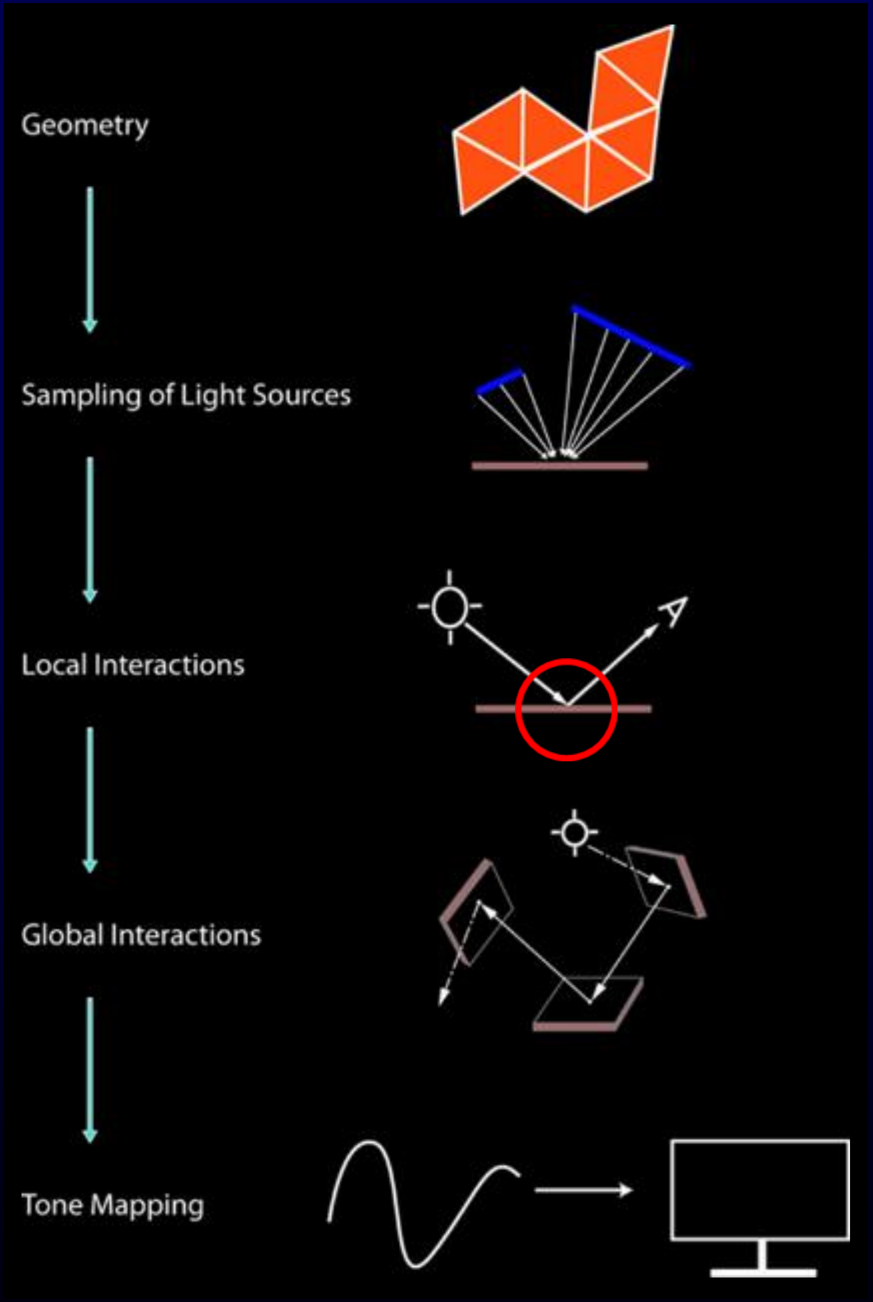


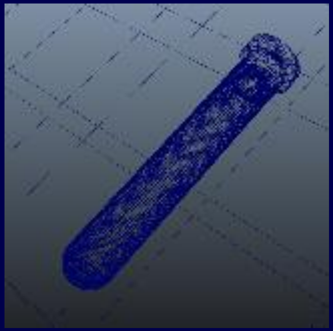
➢ Why do we care about predictability?

- Applications in realistic image synthesis
  - Makes the rendering process more automatic and less dependent on *ad hoc* parameters
  - Facilitates the reproduction of rendering results

How?

Image Synthesis Pipeline





CLBlood

- Applications in life sciences

  - Interpretation of remote sensing data used to:

    - study nutrient cycles within ecosystems

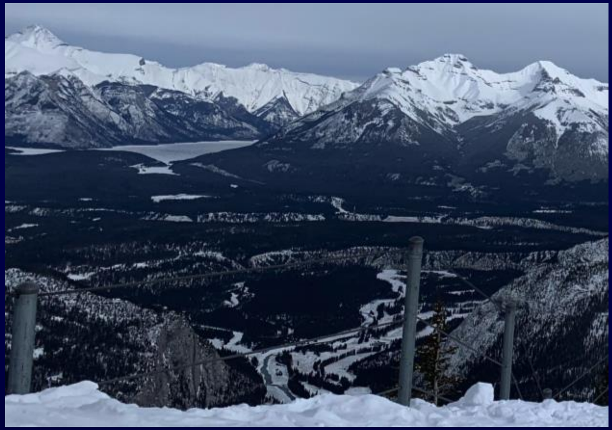
    - assess the biochemistry and water content of regions of vegetation and soils

    - estimate crop productivity

- Study of climate change effects on snow cover

- Study of climate change effects on snow cover

- Assessment of their impact on:
  - ❖ fresh water availability
  - ❖ weather patterns
  - ❖ vegetation greening
  - ❖ avalanche conditions



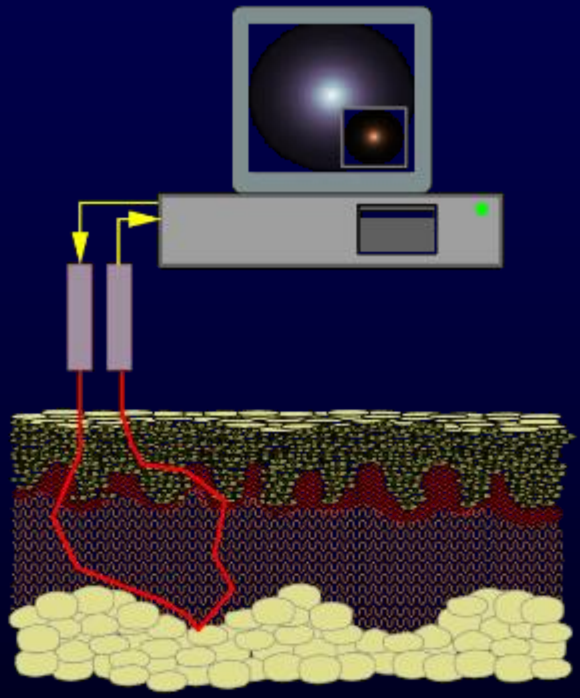
- Applications in health sciences
  - Study of photobiological processes
    - erythema (redness)

- Applications in health sciences
  - Study of photobiological processes
    - erythema (redness)
    - melanogenesis (tanning)

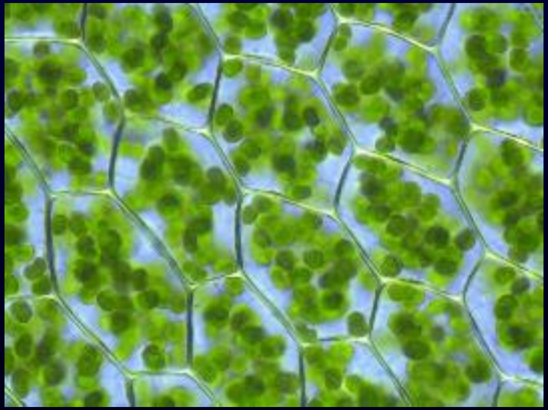
- Applications in health sciences
  - Study of photobiological processes
    - ❖ erythema (redness)
    - ❖ melanogenesis (tanning)
    - ❖ photocarcinogensis (skin cancer)

- Noninvasive measurement of tissue optical properties used in:

  - prevention of diseases
  - diagnostic spectroscopy
  - therapeutic dosimetry

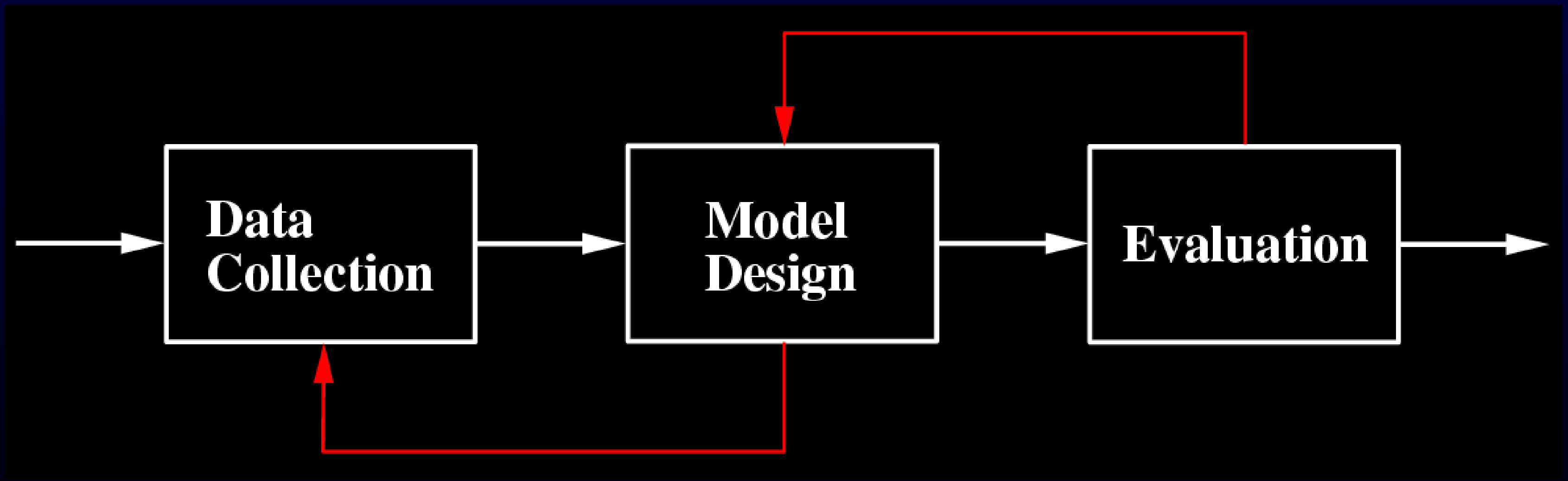


- Investigation of biological phenomena triggered by light
  - Photosynthesis
  - Morphogenesis
  - Phototropism
  - Chloroplast movements



➢ What are the main “ingredients” to achieve predictability?

- Biophysically-based approaches
- Interdisciplinary efforts (cross-fertilization)
- Scientifically sound (model) development frameworks

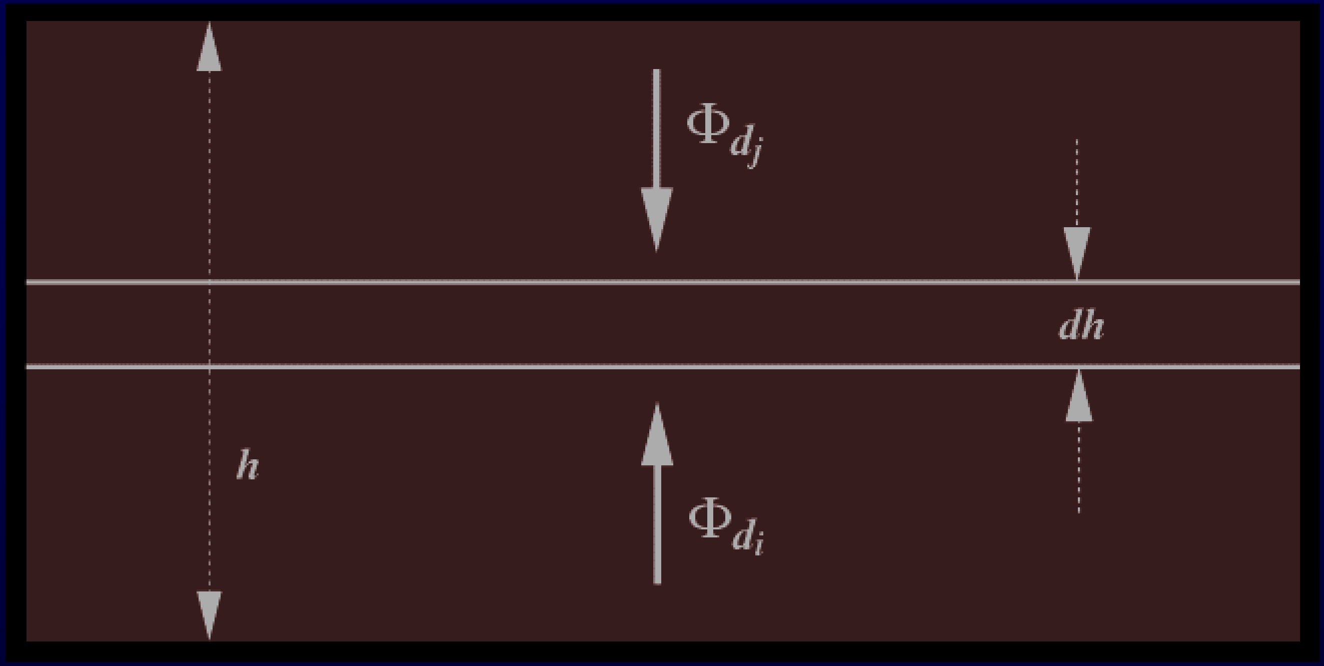


Framework Choices

- Design strategies:
  - Top-down
  - Ground-up (first-principles)
- Simulation approaches:
  - Deterministic (*e.g.*, based on the Kubelka-Munk theory)
  - Non-deterministic (*e.g.*, based on Monte Carlo methods)

➢ Kubelka-Munk theory based algorithms

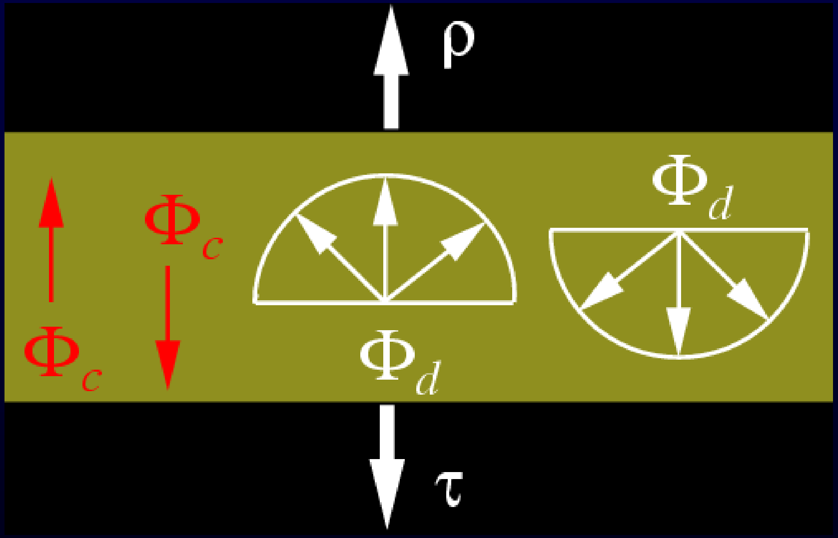
- Kubelka-Munk (K-M) theory (1931)
  - It applies energy transport equations to describe the radiation transfer in diffuse scattering media
  - Parameters: scattering and absorption coefficients
  - Two fluxes: diffuse downward and upward
  - The relations between the fluxes are expressed by linear differential equations



$$-d\Phi_{dj} = -(\mu_a + \mu_s)\Phi_{dj}dh + \mu_s\Phi_{di}dh$$

$$d\Phi_{di} = -(\mu_a + \mu_s)\Phi_{di}dh + \mu_s\Phi_{dj}dh$$

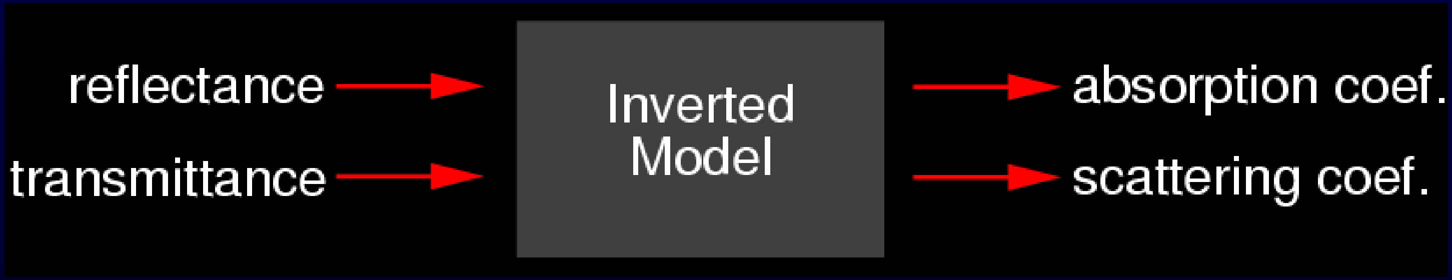
- K-M (flux) approaches used in tissue/environmental optics
  - Use K-M equations relating tissue optical properties to measured reflectance and transmittance values
  - Expand the K-M formulation by adding more coefficients and fluxes



- Pros and cons

  - Enable the rapid determination of optical properties (*e.g.*, absorption and scattering coefficients) through inversion procedures:

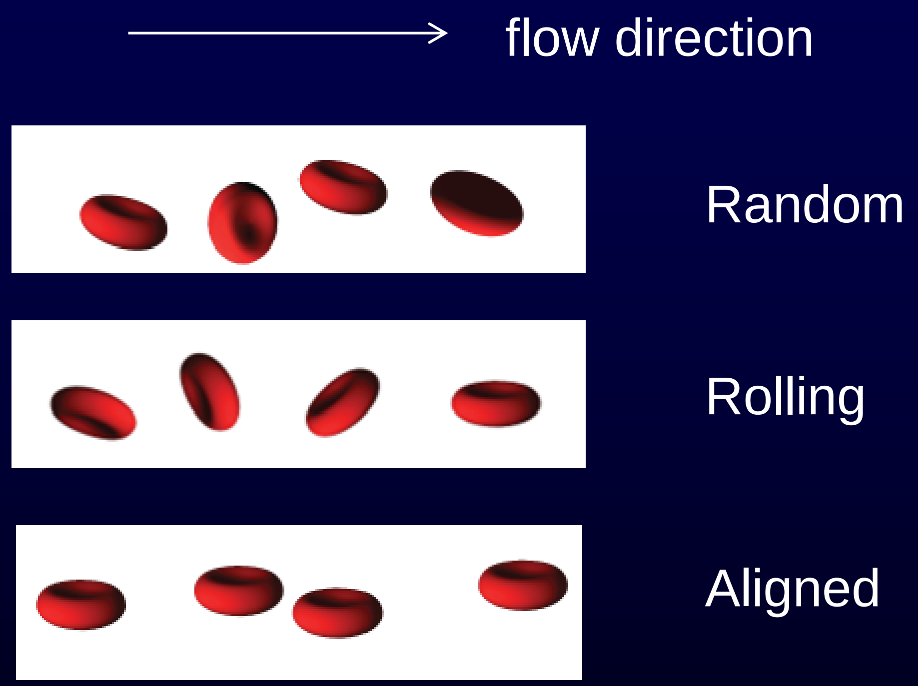
    - ❖ a way to derive biochemical and optical properties from *in situ* and noninvasive measurements



  - Have a limited applicability to the computation of BRDF and BTDF

  - Lack the flexibility to account for specific material characteristics

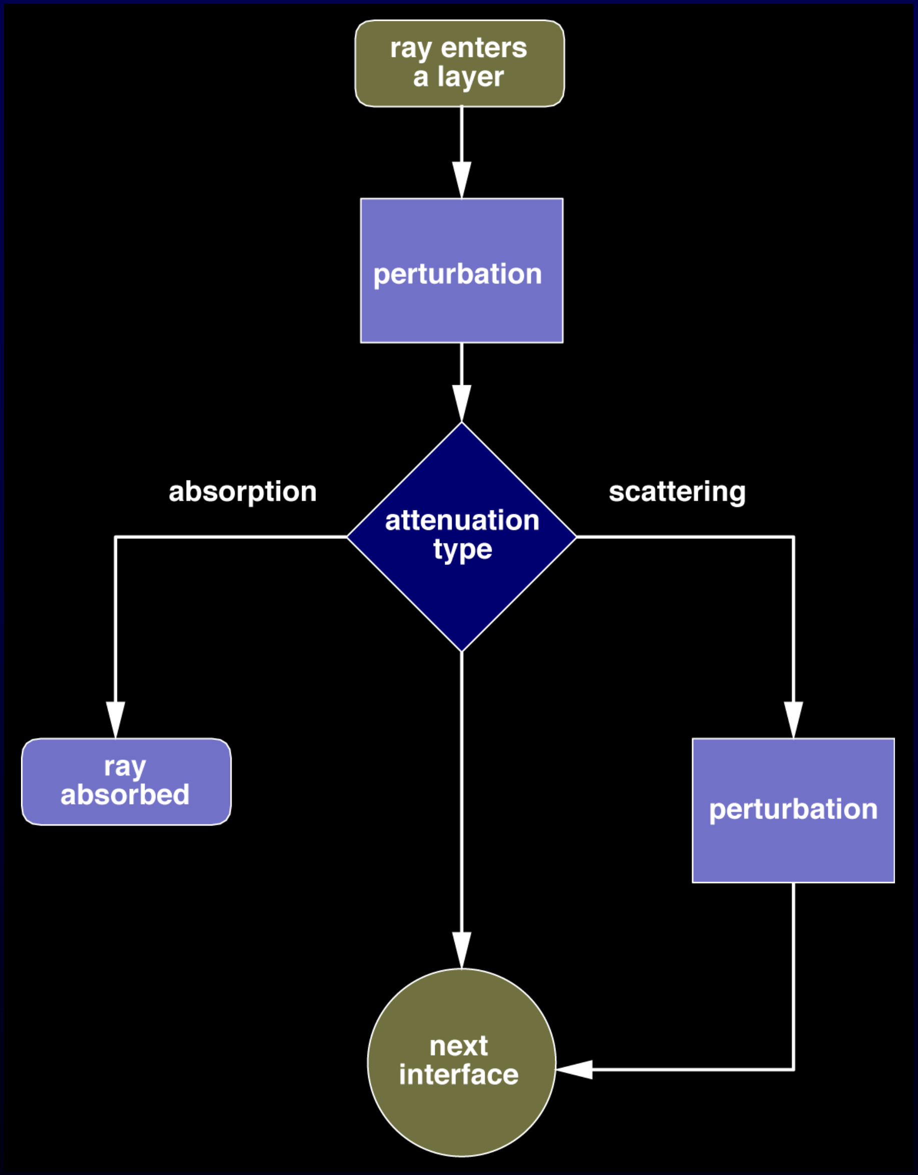
❖ Example: rheological states affecting the optical properties of whole blood



Monte Carlo based algorithms

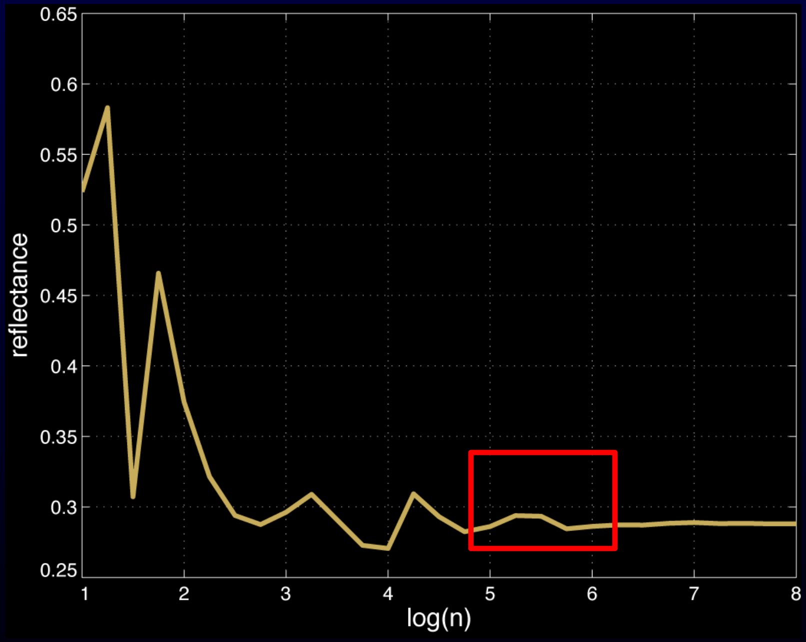
- Monte Carlo approach
  - Originally proposed by Metropolis and Ulam (1949) to stochastically simulated radiative transfer processes
  - Idea: to keep track of photons' histories (random walks) as they are scattered or absorbed within a material or environment
  - Extensively employed in many fields

Example:


ray enters a layer
perturbation
absorption
attenuation type
scattering
ray absorbed
perturbation
next interface

- Pros and cons
  - Sufficiently flexible to allow the simulation of local and global light interactions with complex materials within distinct environments
  - The correctness of the simulations is bounded by the plausibility of the input parameters and the proper representation of the scattering and absorption mechanisms
  - Computationally intensive

How many samples (*n*) do we need?



Schedule

- ✓ Introduction
- ✓ Biophysical Background
- ✓ Drawing Board
- ❑ Data Availability and Quality

Break

- ❑ Design Issues
- ❑ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

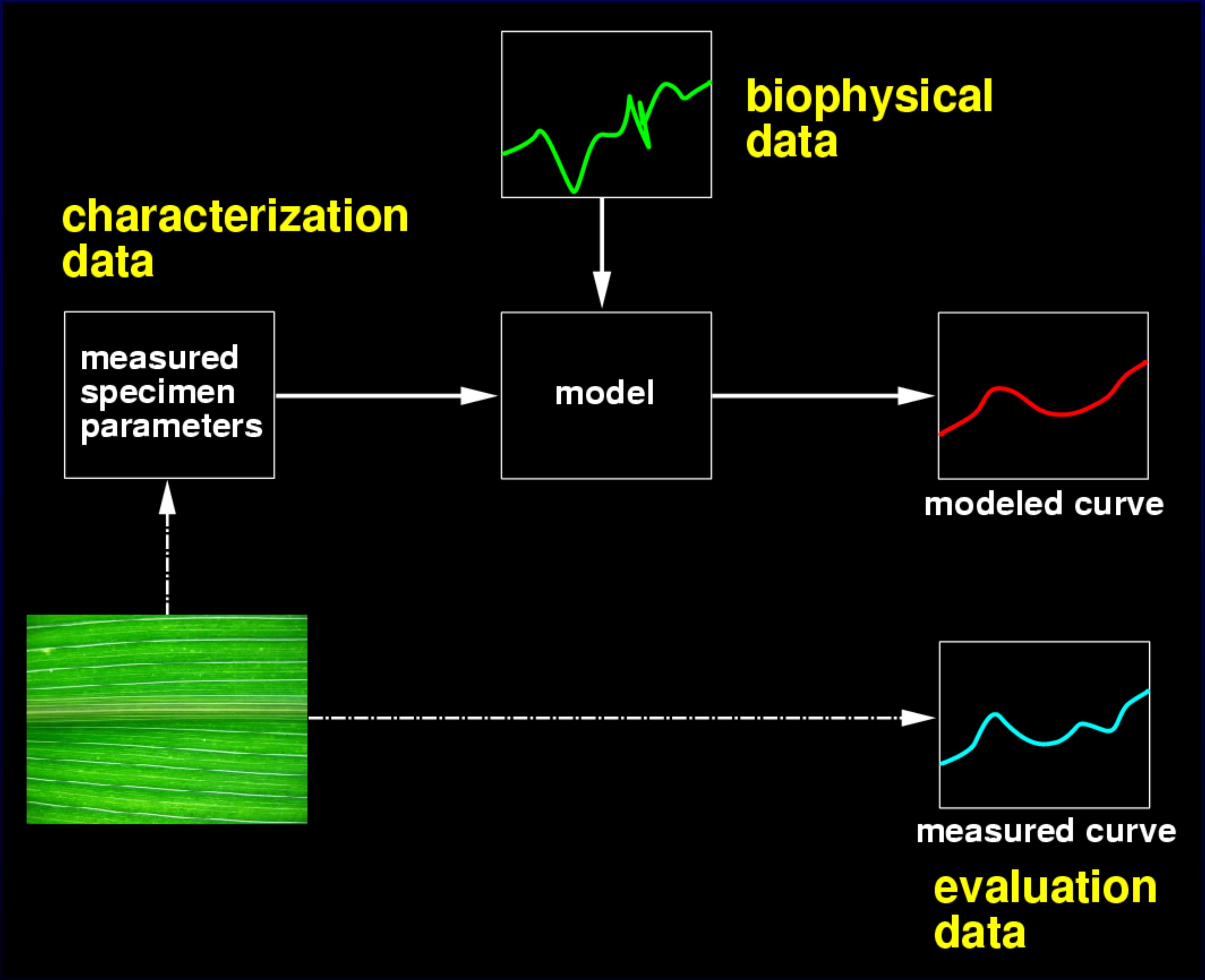
Data Availability and Quality

- Biophysical Data Constraints
- Characterization Data Constraints
- Evaluation Data Constraints

"Good science requires both theory and data – one is of little use without the other."
G. Ward (1992)

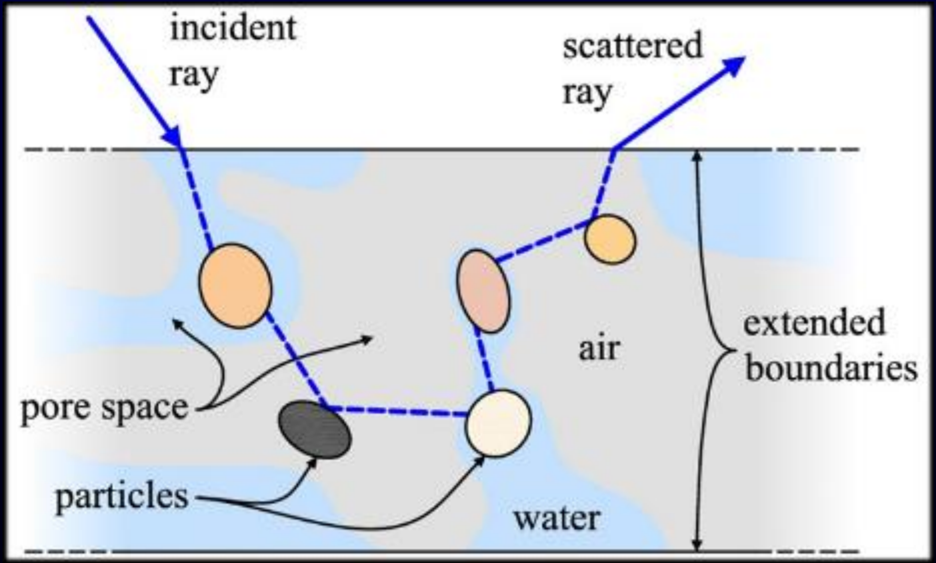
➢ In our case, what data?

- Biophysical data
  - Refractive indices, absorption coefficients, etc …
- Characterization data
  - Thickness, concentration of pigments, etc …
- Evaluation data
  - Reflectance, transmittance, BRDF, etc …

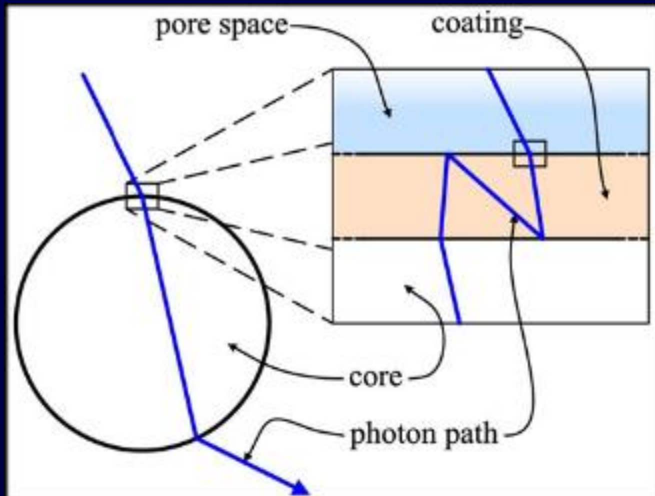

biophysical data
characterization data
measured specimen parameters
model
modeled curve
measured curve
evaluation data

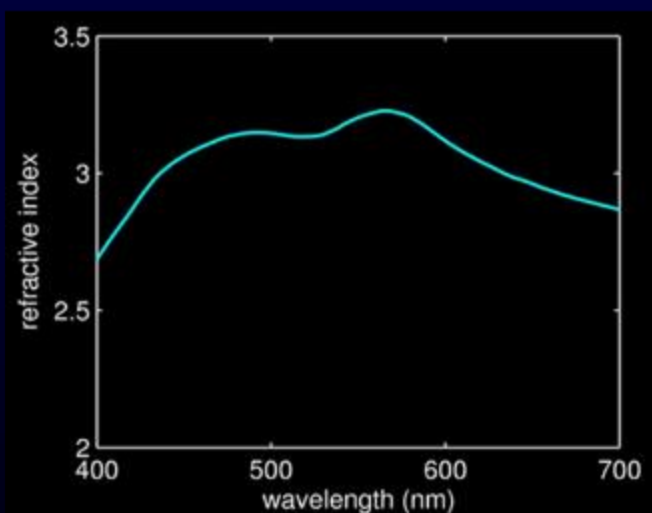
Biophysical Data Constraints

- Scarcity
  - Spectral refractive indices (real and complex)
    - Example: simulation of light interactions with sand

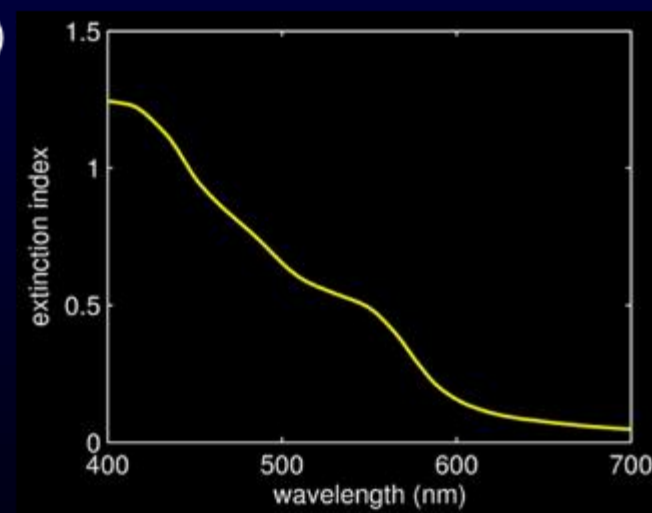


SPLITS



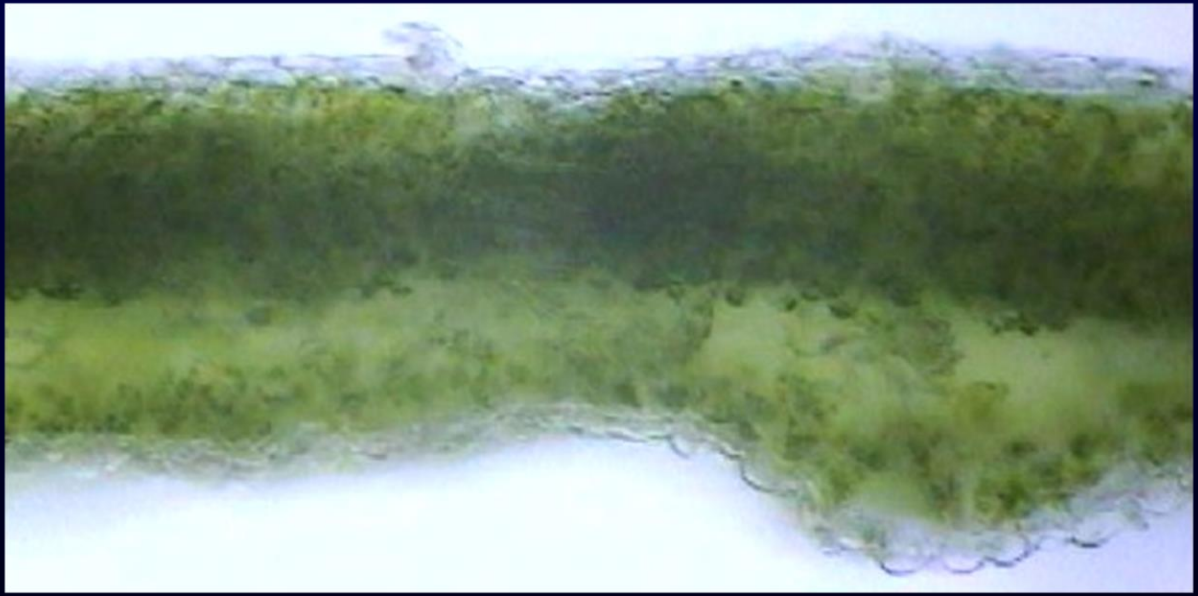


Hematite (red ochre)



- Often, only average single values are available in the literature
    - ❖ for example, mesophyll of soy leaves = 1.42

Leaf Cross-Section



- Although Gladstone and Dale law can be used to obtain spectral indices, it also suffers from data unavailability issues

$$\eta(\lambda) = c_s \eta_s(\lambda) + (1 - c_s)\eta_b(\lambda)$$

where:

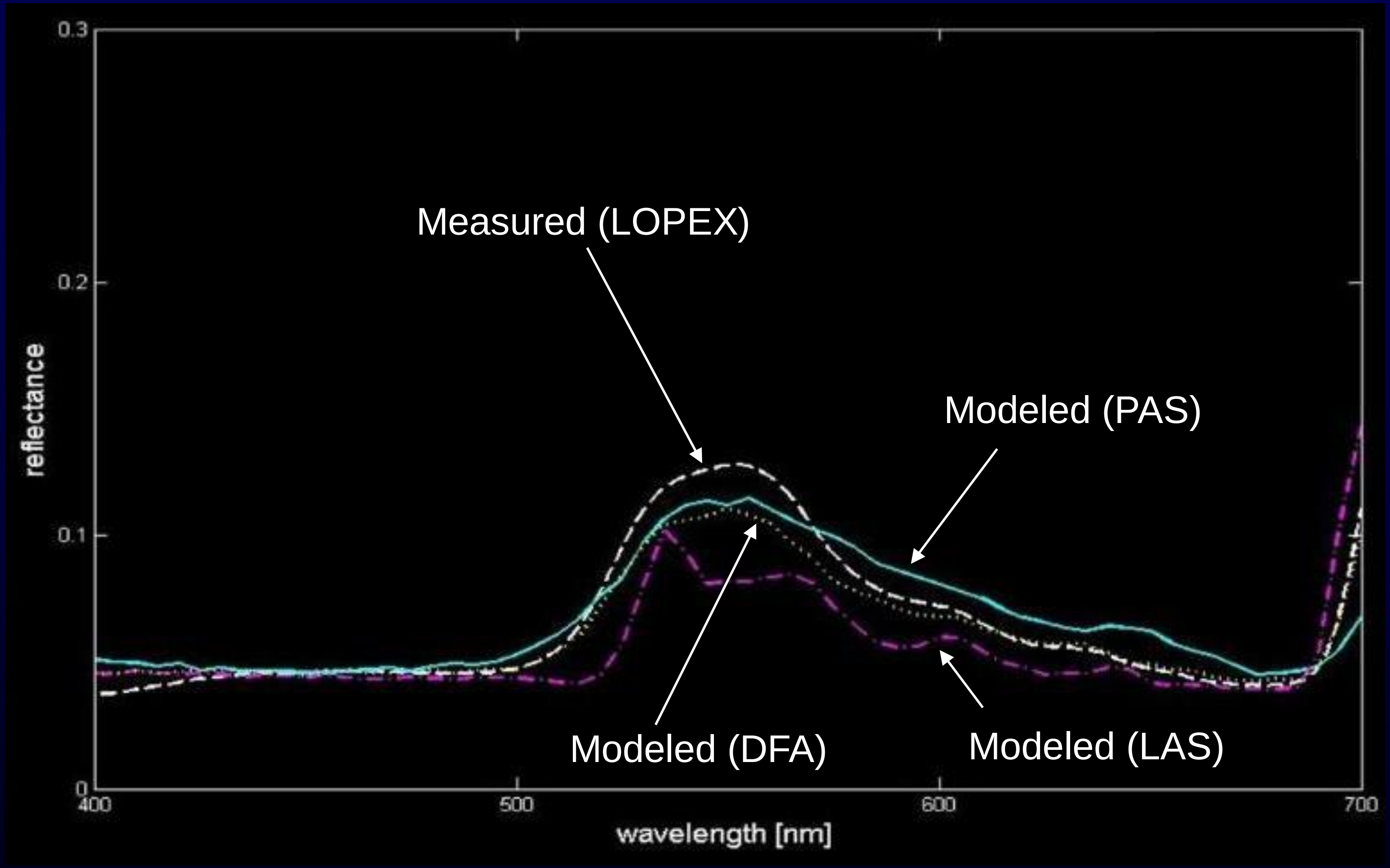
c_s = volume fraction of scatterers,

η_s = refractive index of the scattering material,

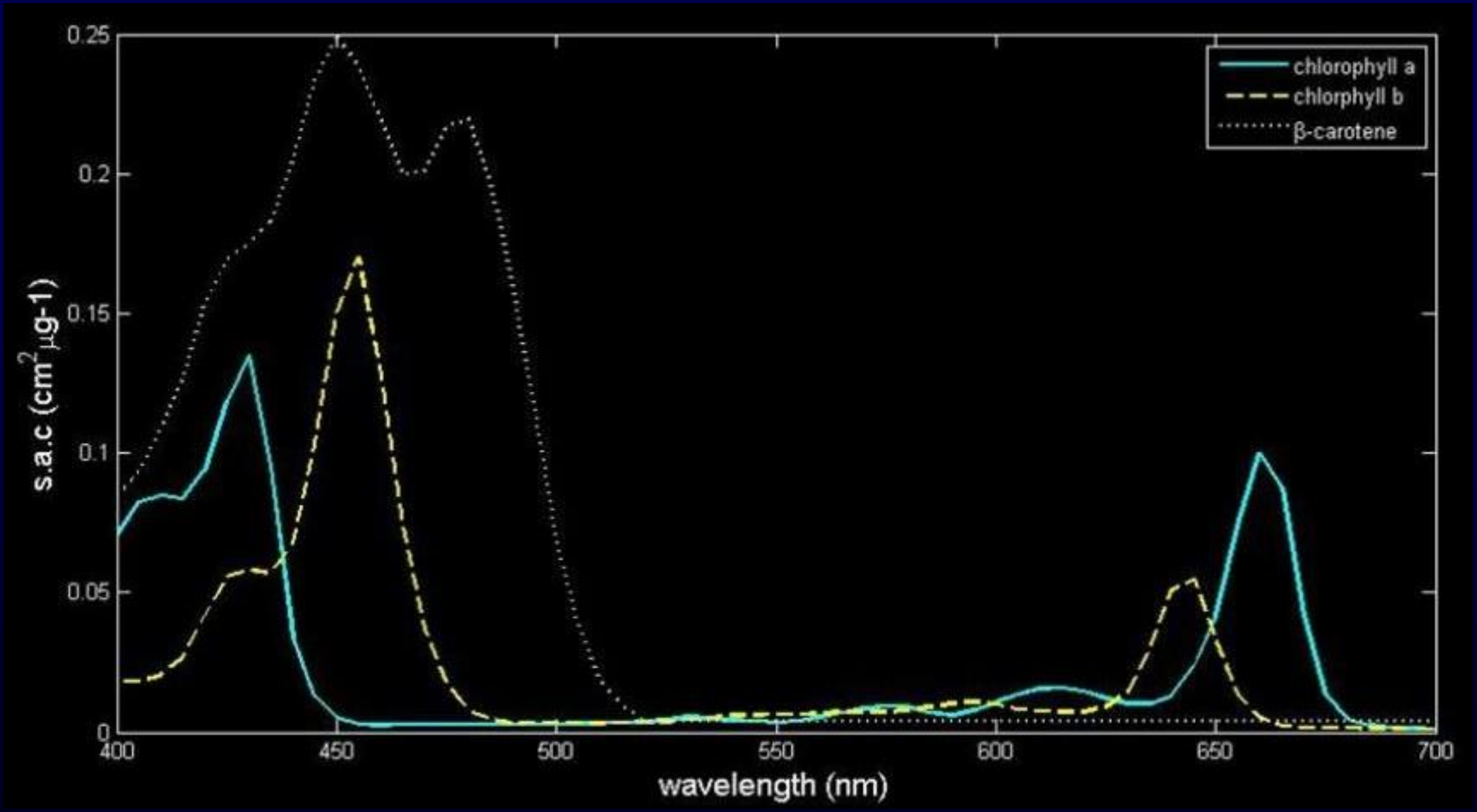
η_b = refractive index of the base material.

- Specific absorption coefficients
  - Example: “the chlorophyll case”

Measured and Modeled (ABM-B) Reflectance Curves of a Soy Leaf

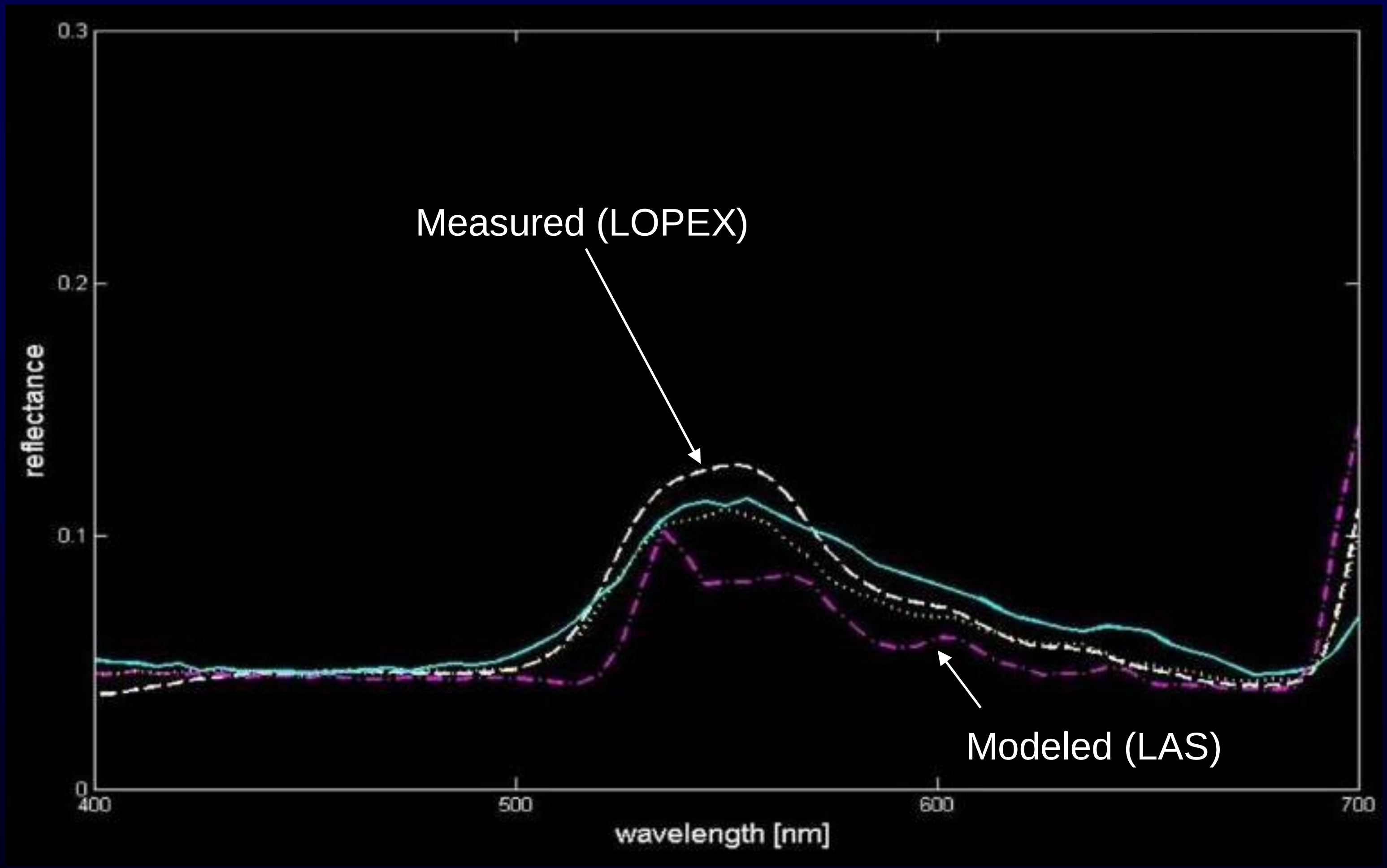


Light Absorption Spectroscopy (LAS)

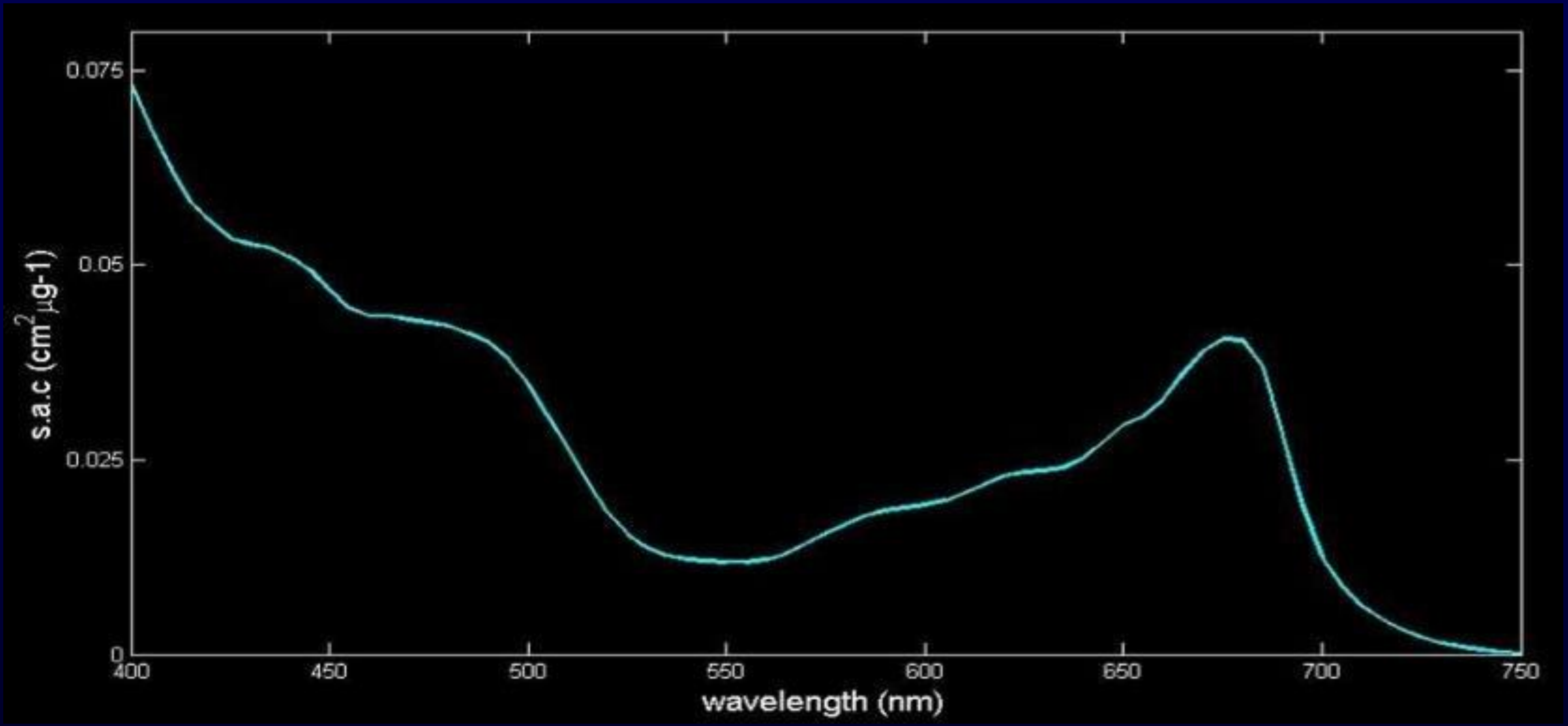


Light Absorption Spectra
(Zscheile and Comar, Botanical Gazette 1941,
Zscheile *et al.,* Plant Physiology 1942)

Measured and Modeled (ABM-B) Reflectance Curves of a Soy Leaf

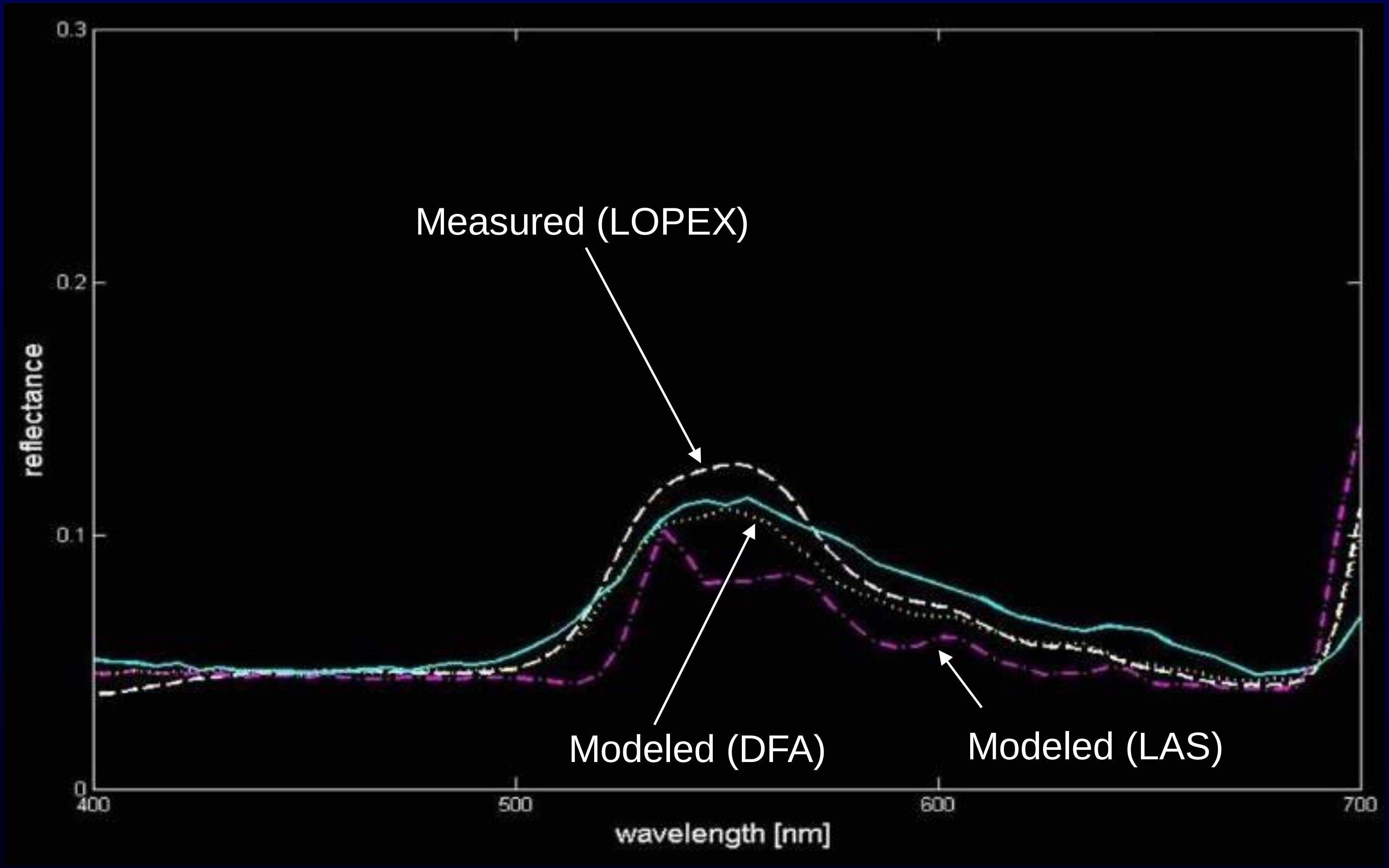


Data Fitting Approach (DFA)

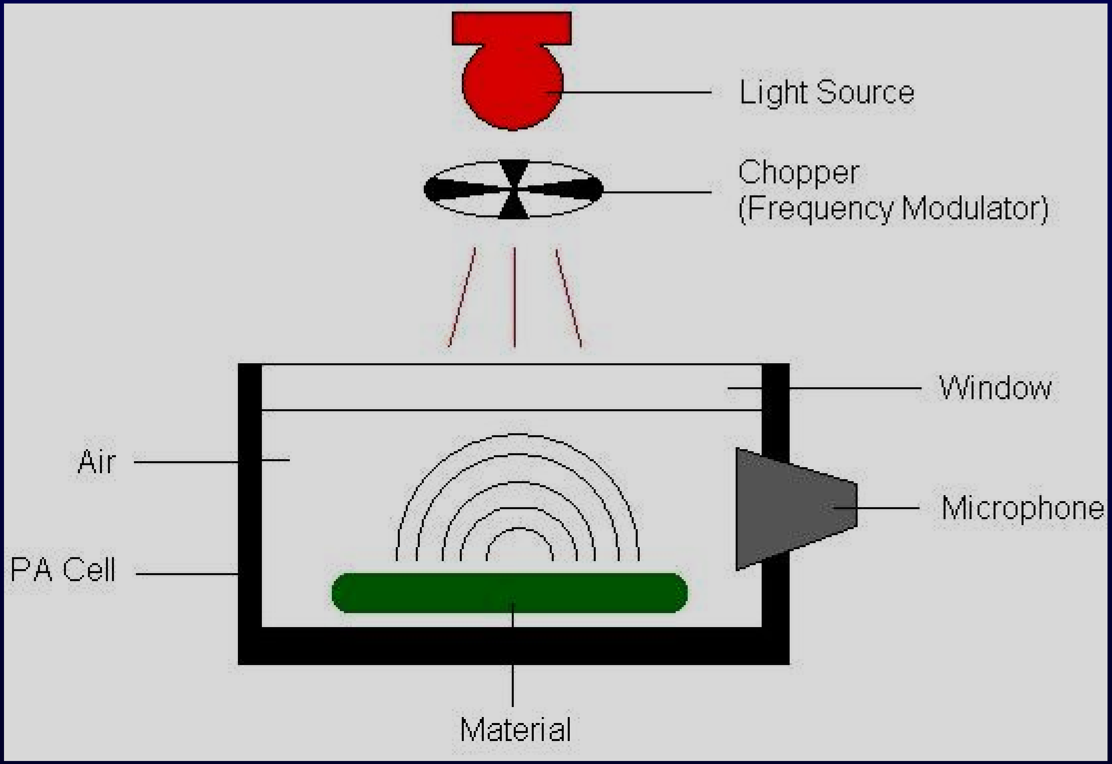


DFA Absorption Spectra for chlorophyll *a+b*
(Jacquemoud *et al.*, Remote Sensing of Environment 1996)

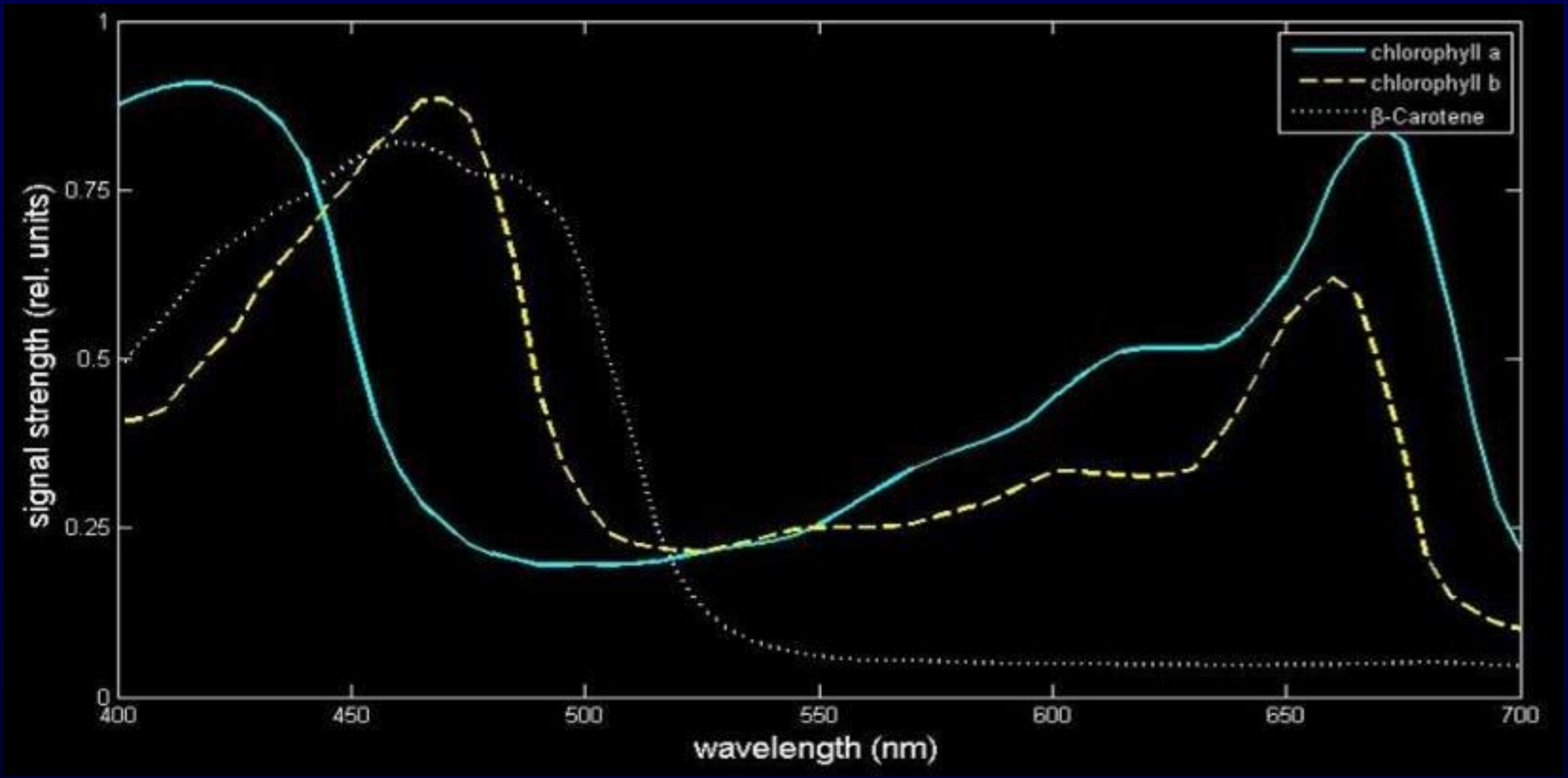
Measured and Modeled (ABM-B) Reflectance Curves of a Soy Leaf



Photoacoustic Absorption Spectroscopy (PAS)

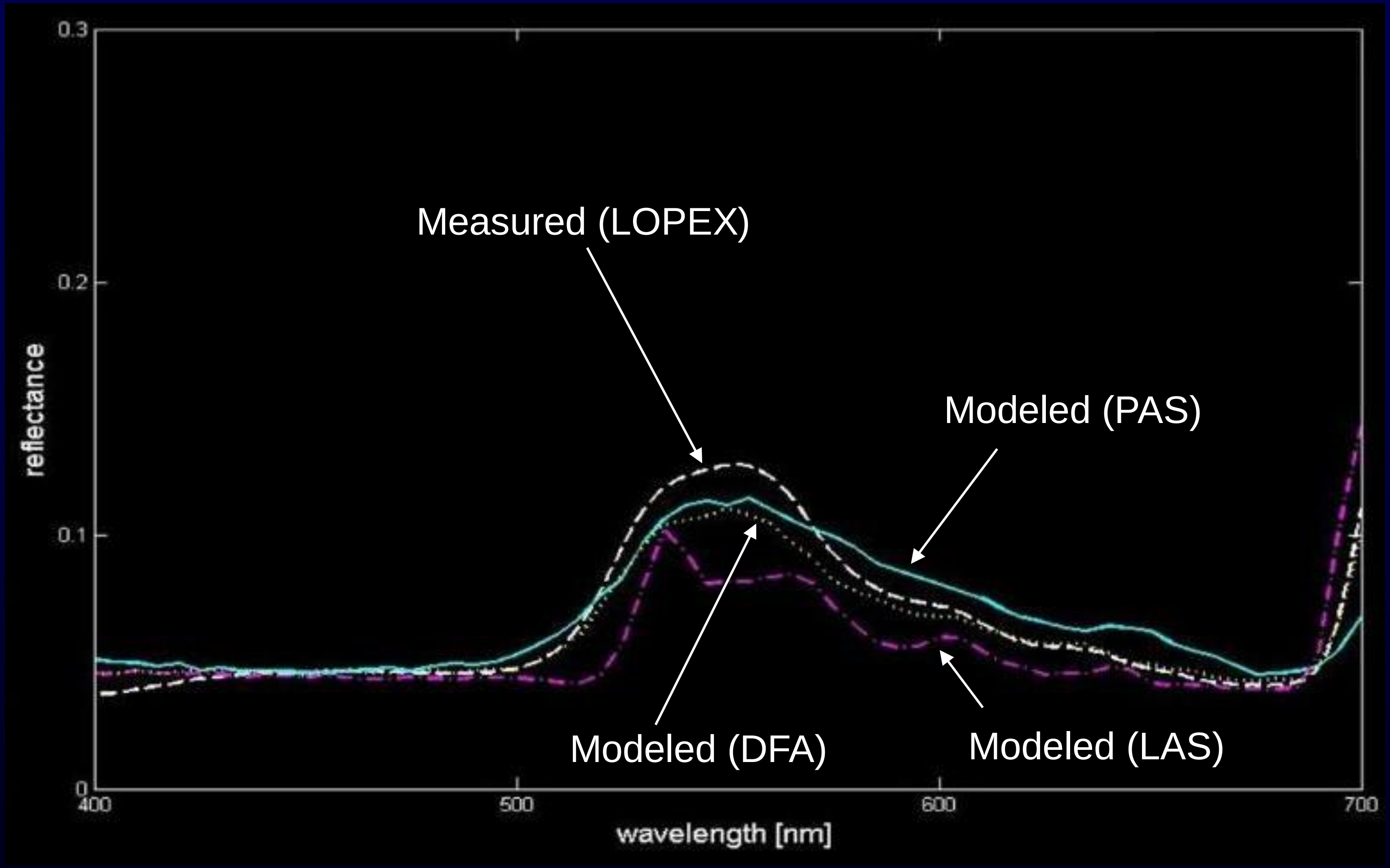


Photoacoustic Spectrometer



Photoacoustic Absorption Spectra
(Nagel *et al.*, *Biological Role of Plant Lipids* 1989)

Measured and Modeled (ABM-B) Reflectance Curves of a Soy Leaf



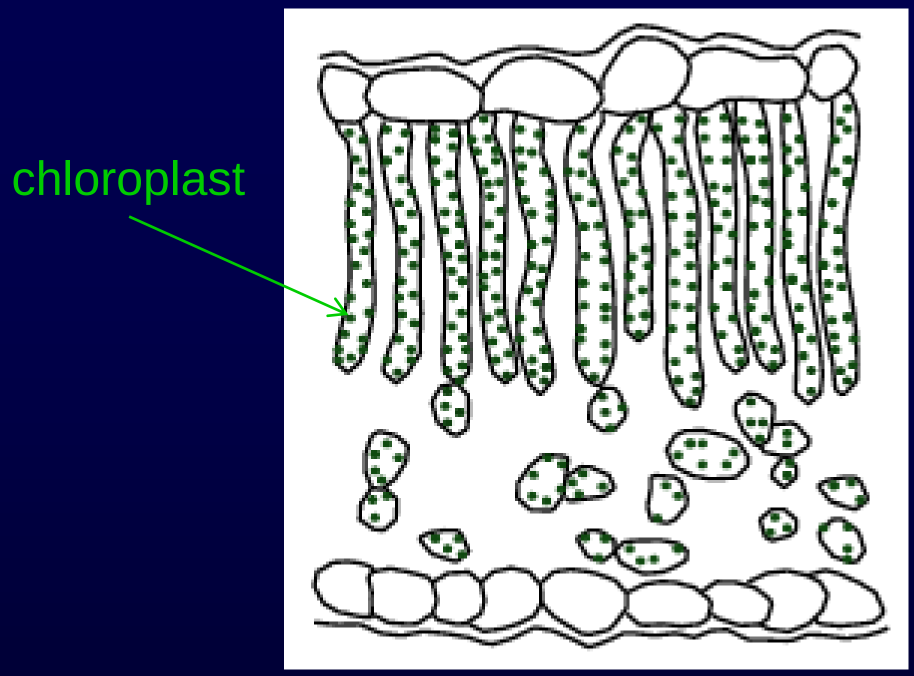
➢ Reliability issues: *in vivo* vs. *in vitro*

→

In vivo pigments

In vitro pigments

Cross-Section of a Plant Leaf

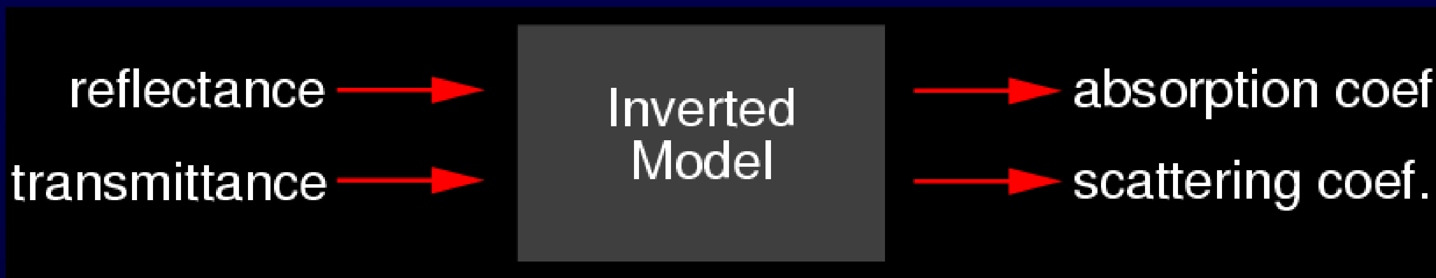


Chlorophyll Solution

- Sieve and detour effects

- Spectral shifts

- Recall biophysical data derived from inversion procedures

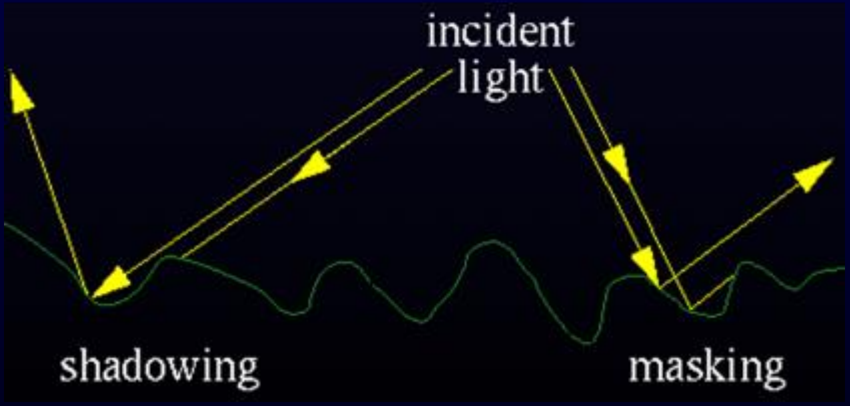


Was the model fully evaluated?

Characterization Data Constraints

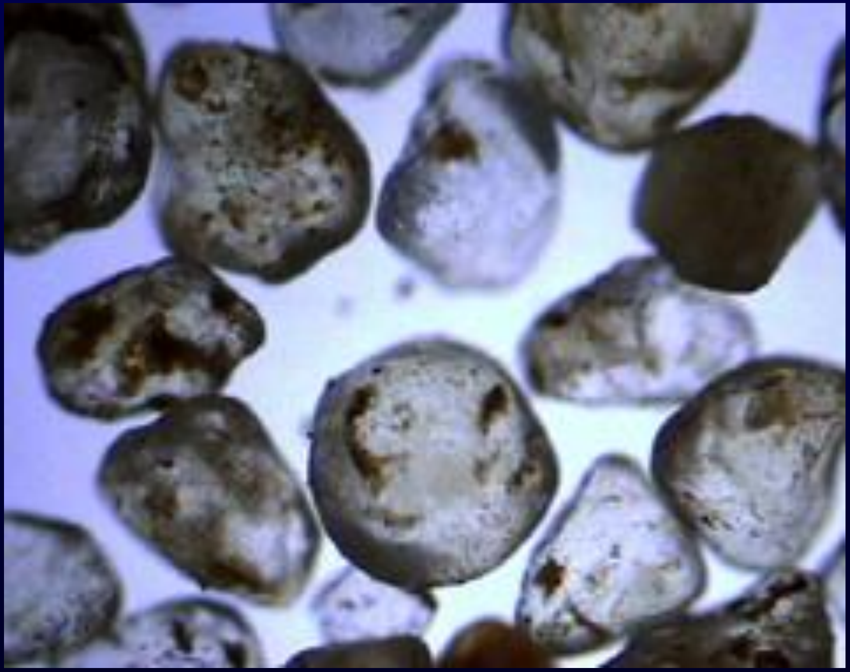
- Scarcity
  - Structural parameters affecting light and matter interactions

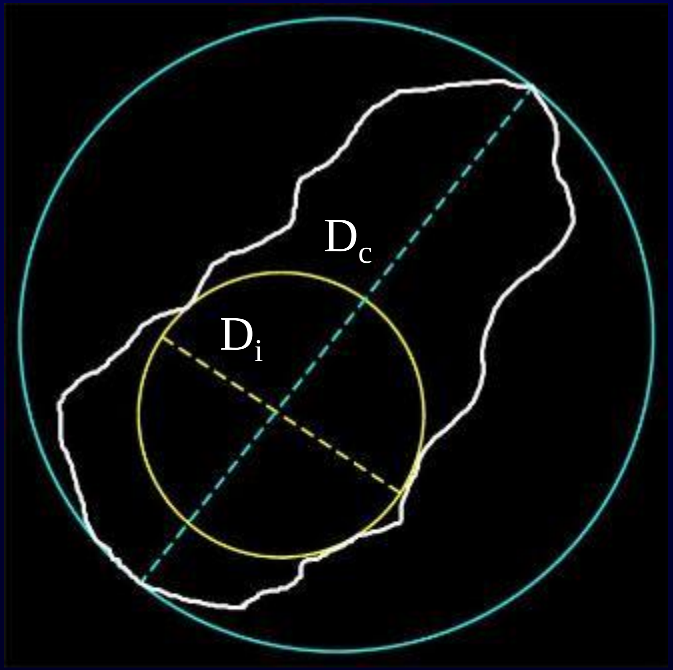
Skin Surface



- Venation systems and hairs

- Sand grains (dimensions, shape and roundness)

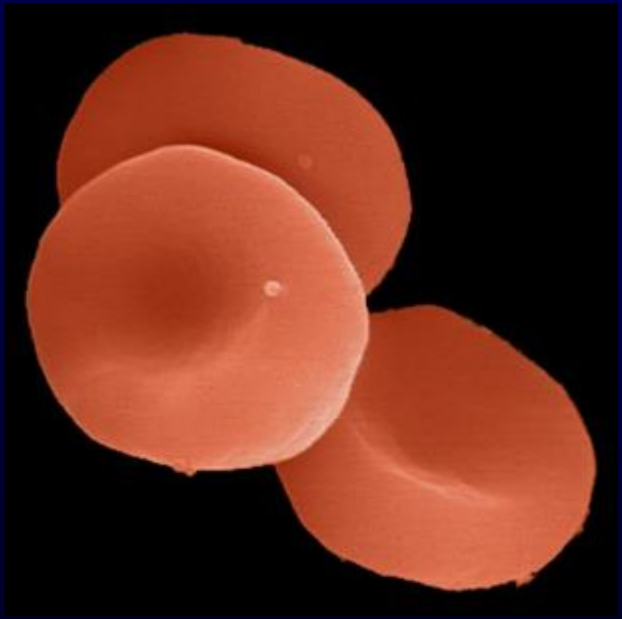




sphericity = sqrt (D_i/D_c)

- Red blood cells (volume, pigment content and scattering profile)

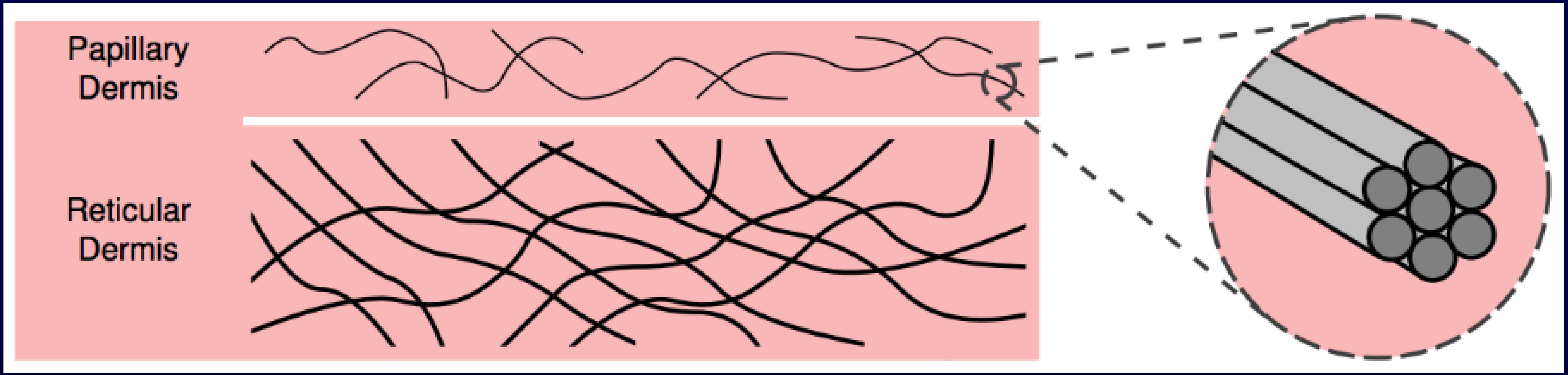
RBCs (SEM)



RBC Cross-Section (sketch)

- Organelles, fibers and fibrils (size, distribution, scattering profile)

Cutaneous Collagen Fibers and Fibrils

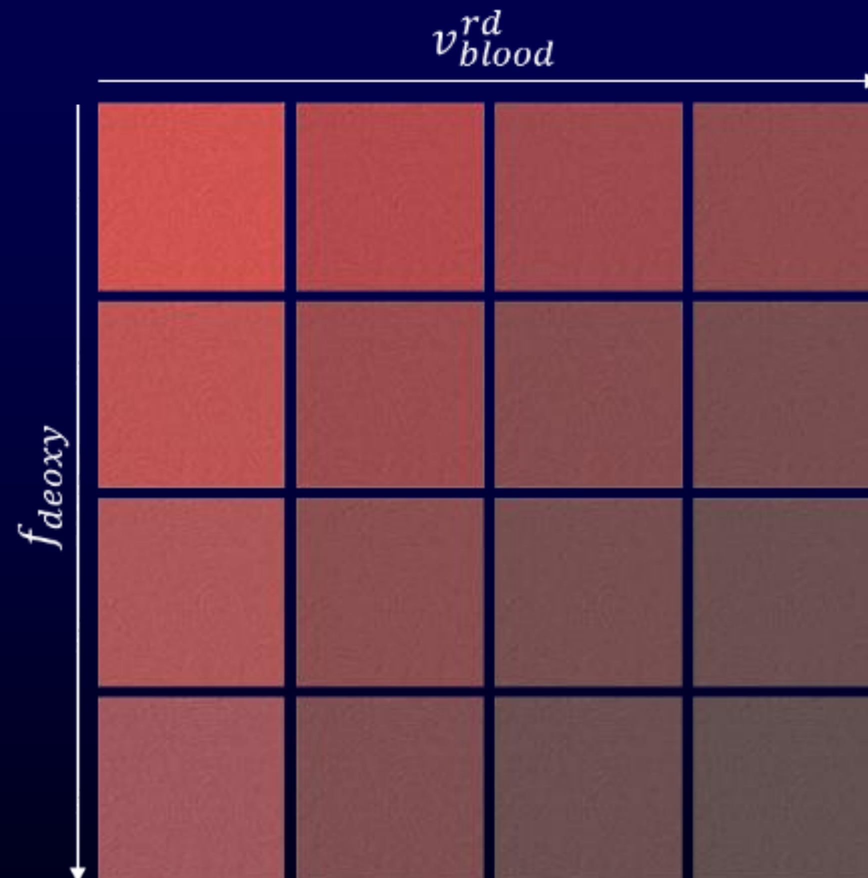


size?

❖ How much impact can something so small have?

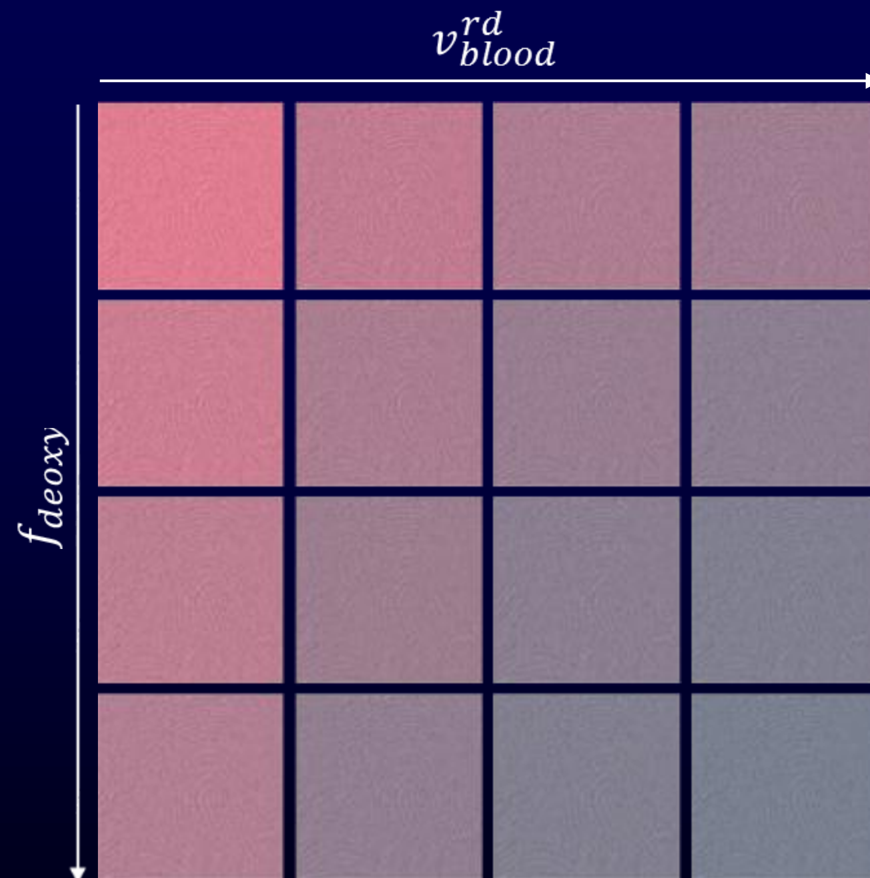
Rayleigh scattering deactivated

Peripheral Cyanosis
(IEEE EMBC 2017,
Biomed. Opt. Exp. 2018)



swatches generated using illuminant D65

Rayleigh scattering deactivated



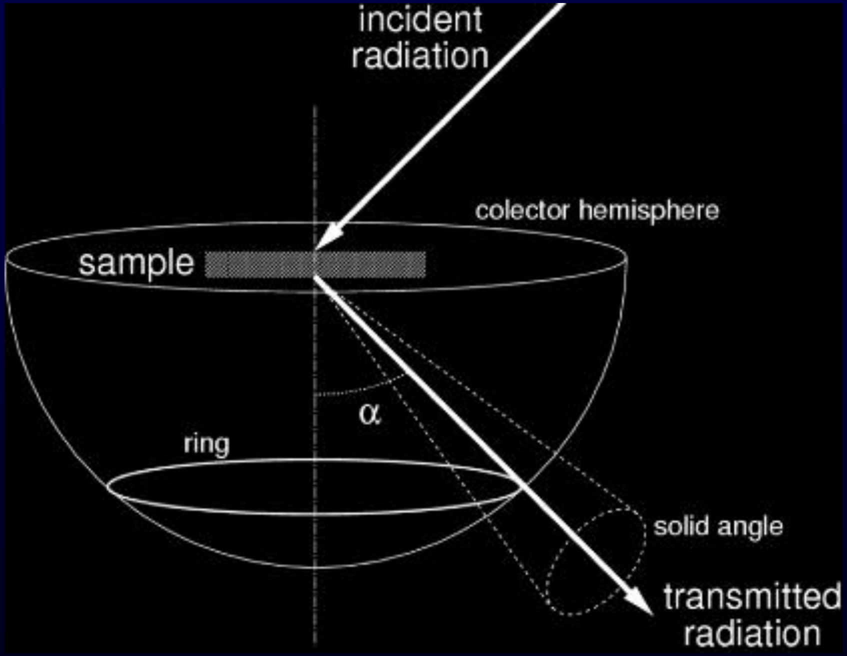
Peripheral Cyanosis
(IEEE EMBC 2017,
Biomed. Opt. Exp. 2018)

swatches generated using
illuminant D65

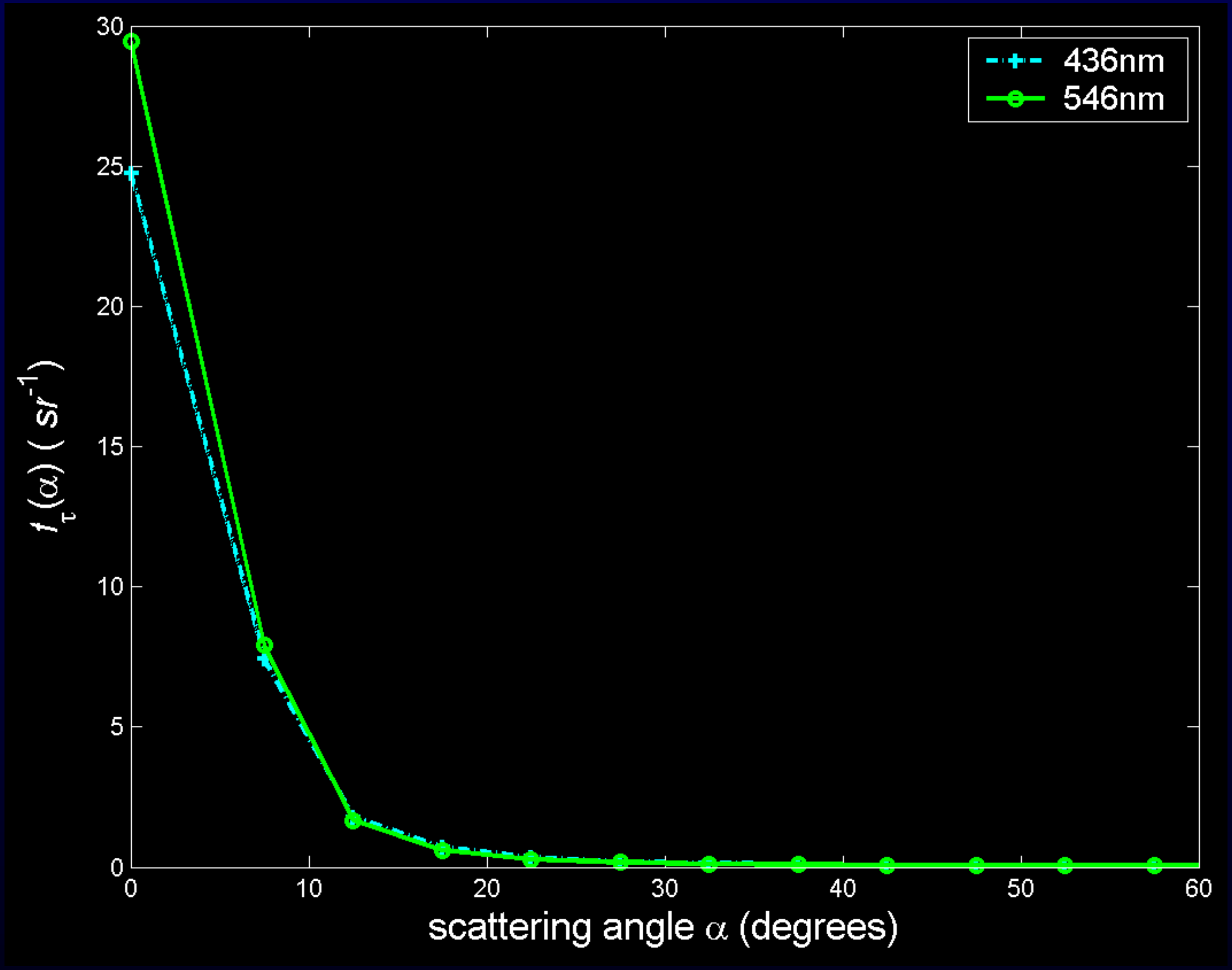
- Material subsurface scattering data

- Subsurface scattering data is usually limited to a few wavelengths

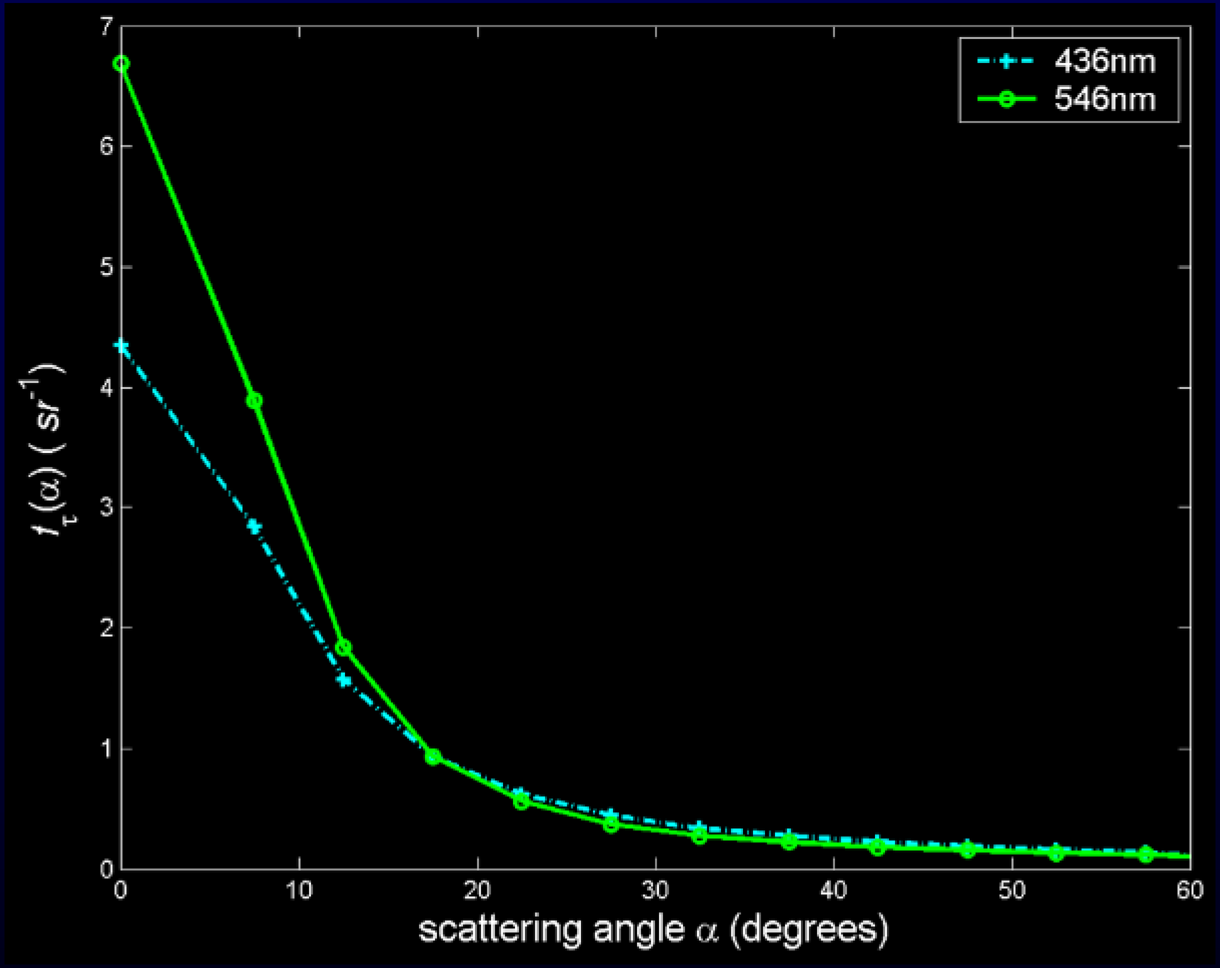
  ❖ Example: skin subsurface measurements performed by Bruls and van der Leun (1984)



❖ Stratum corneum

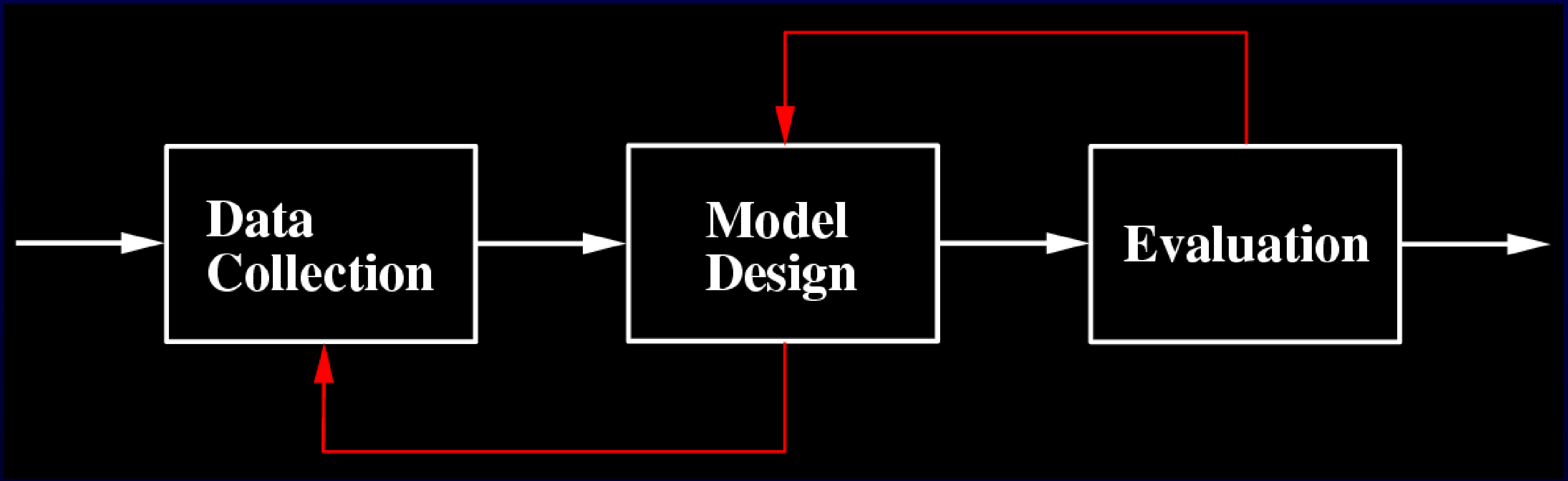


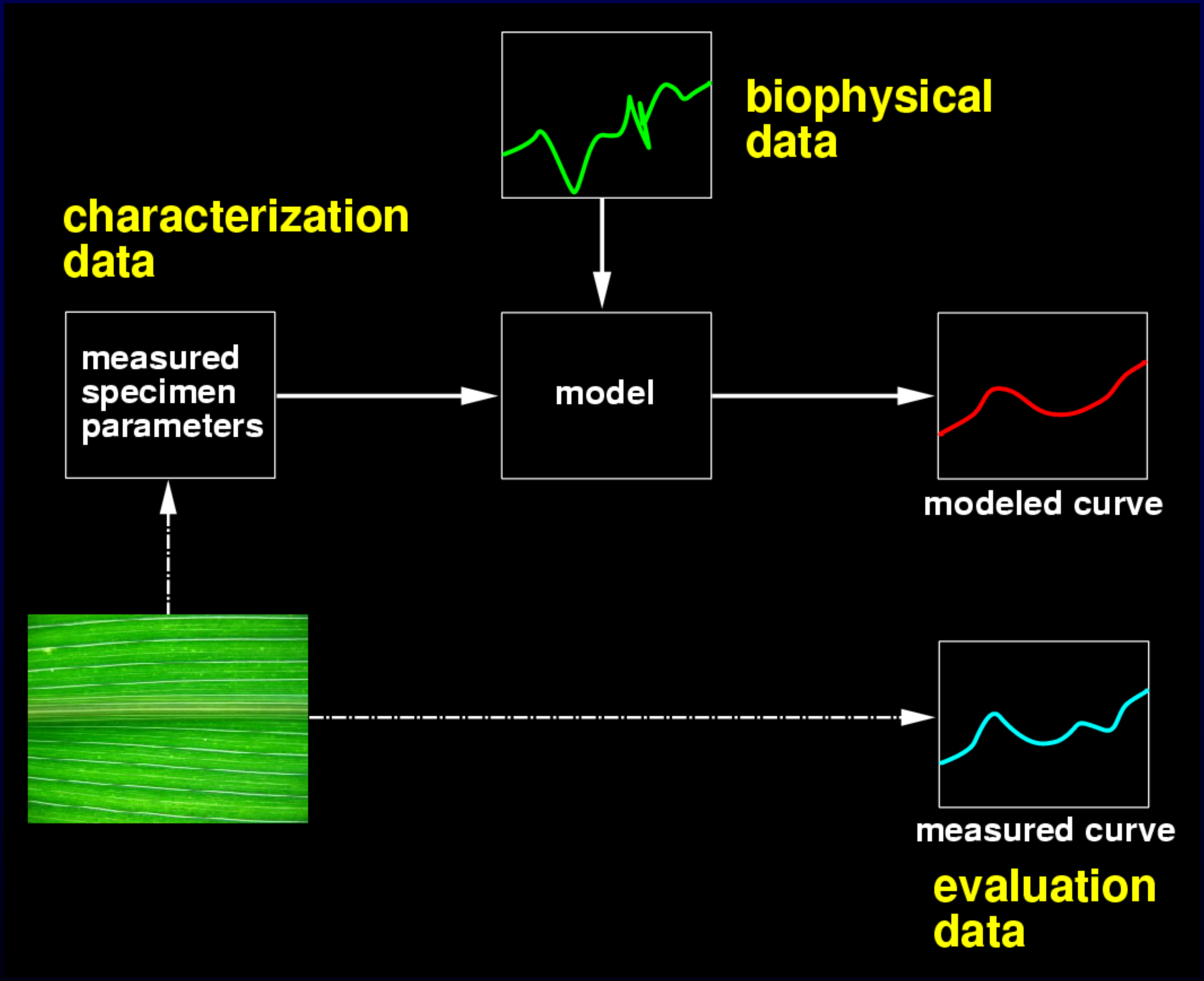
❖ Epidermis



436nm
546nm
$f_\tau(\alpha)$ (sr^{-1})
scattering angle α (degrees)
0
1
2
3
4
5
6
7
0
10
20
30
40
50
60

Evaluation Data Constraints




biophysical
data
characterization
data
measured
specimen
parameters
model
modeled curve
measured curve
evaluation
data

Reality Check

- Measured spectral data (*e.g.*, reflectance, transmittance and BSDF) is scarcely found in the literature

- Available spectral databases rarely include comprehensive characterization data associated with the employed samples and specimens

- Noteworthy counter-examples:

  - LOPEX (Leaf Optical Experiments)

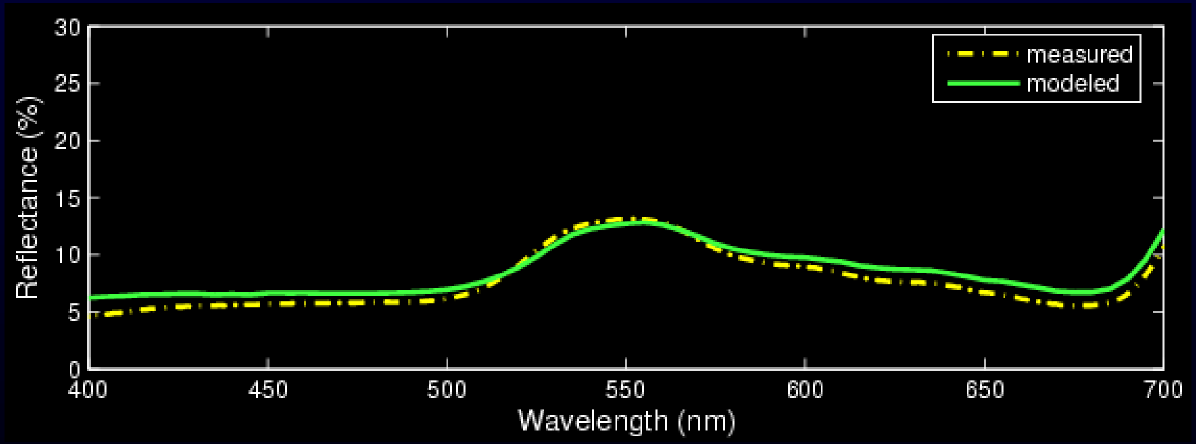
  - SISpec (Snow & Ice Spectral Libray)

- LOPEX spectral data (reflectance and transmittance) is accompanied by the leaf specimens':

  ❖ thickness

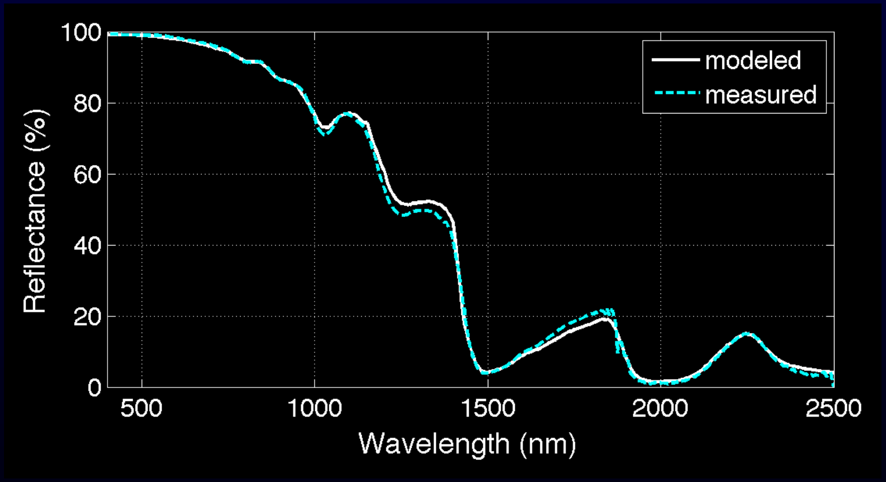
  ❖ fresh and dry weights

  ❖ concentration of absorbers (chlorophylls, carotenoids, cellulose, lignin and protein)

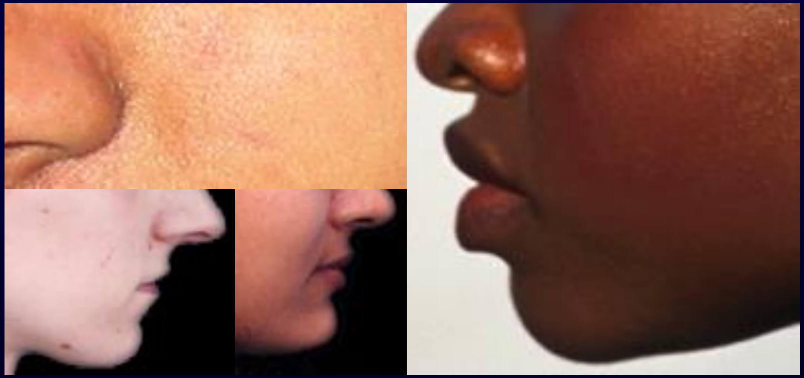


- SISpec spectral data (reflectance) is accompanied by the snow samples':

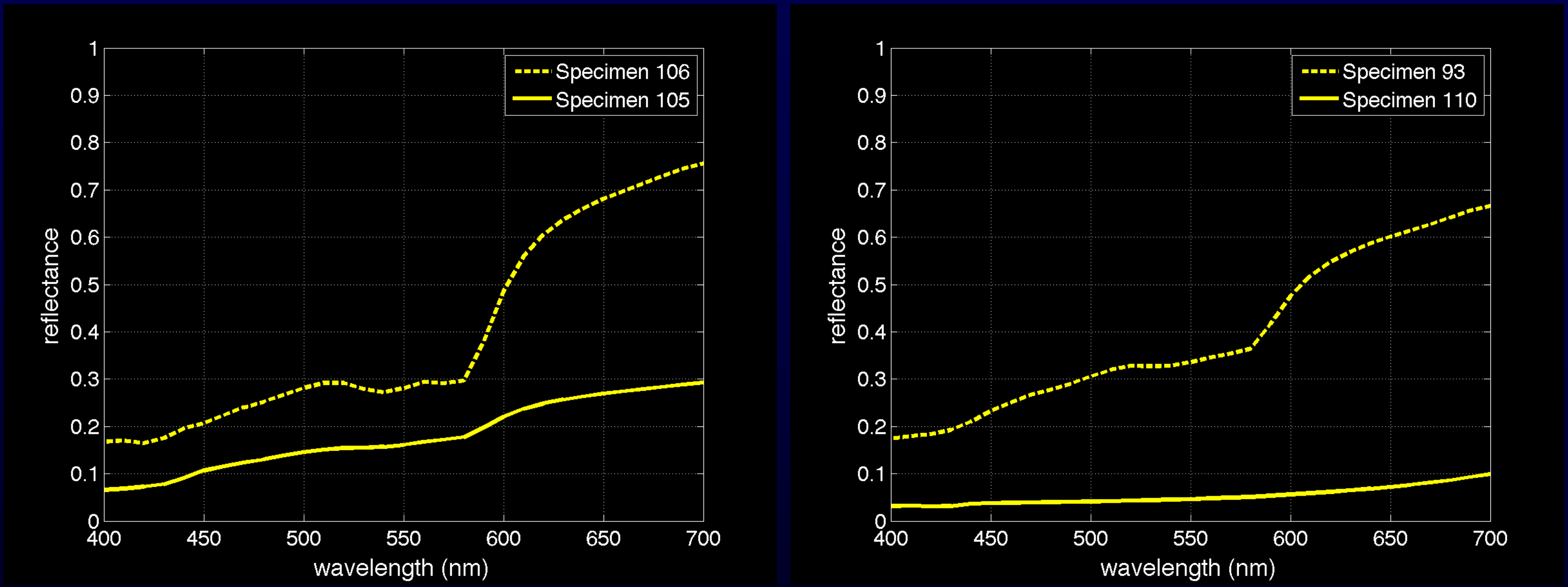
  - ❖ thickness (depth) and temperature
  - ❖ grain size and shape
  - ❖ density and free water content



- In general, only qualitative descriptions are provided
  - How these descriptions really relate to material parameters?
    - Example: human subjects and pigmentation
      - African
      - Caucasian
      - Indian
      - Asian

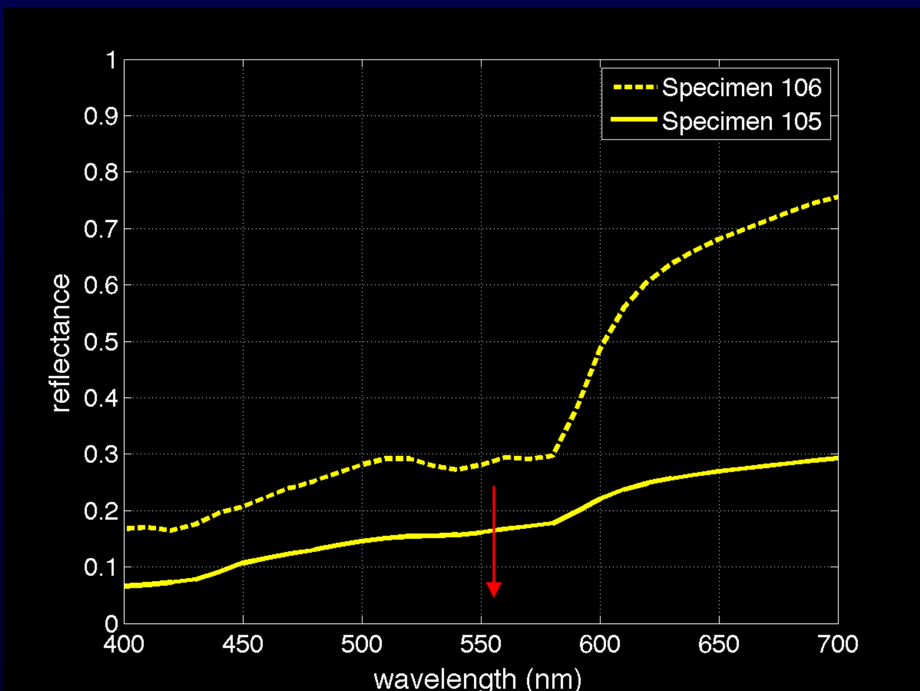


Which of these curves correspond to Caucasian and African specimens?

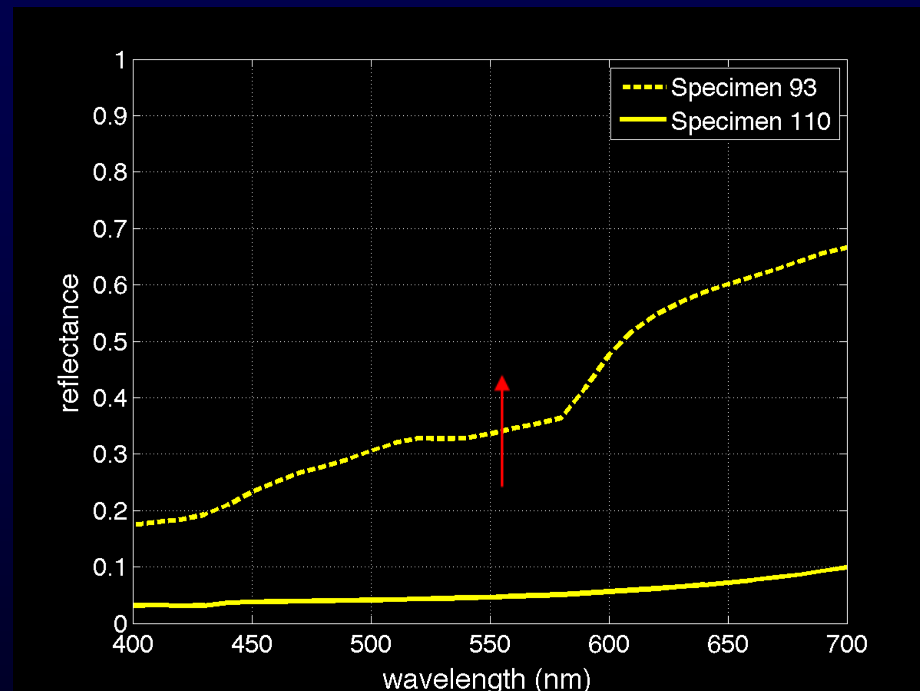


(Vrhel *et al.*, Color Res. Appl. 1994)

Caucasian specimens



African specimens



(Vrhel *et al.*, Color Res. Appl. 1994)

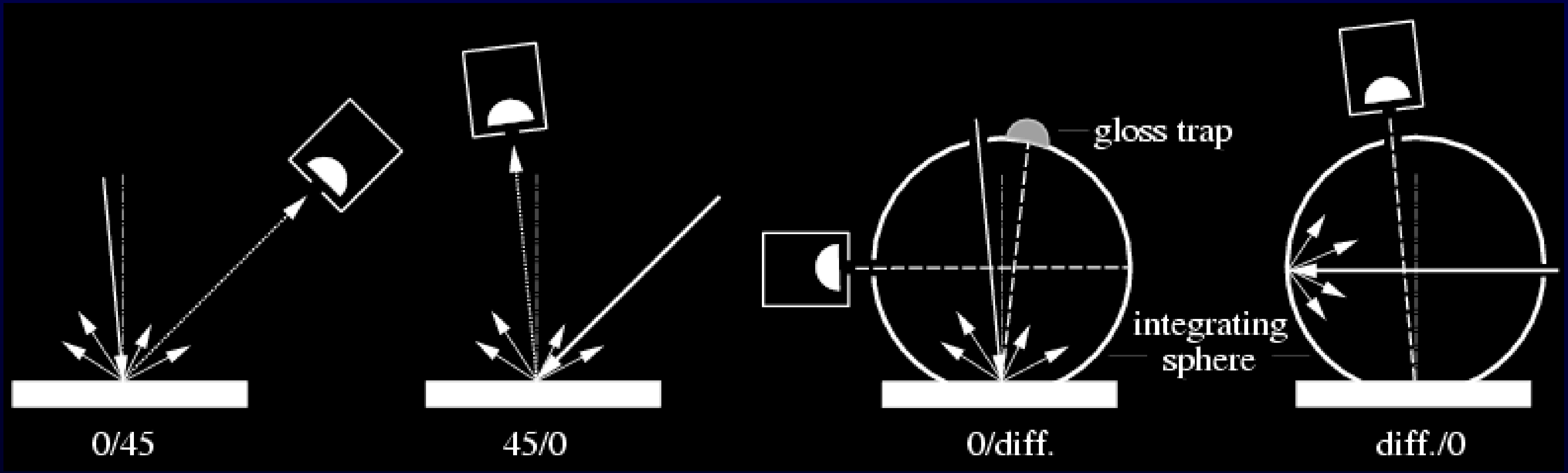
How about tanned specimens?

Facultative Pigmentation

Constitutive Pigmentation

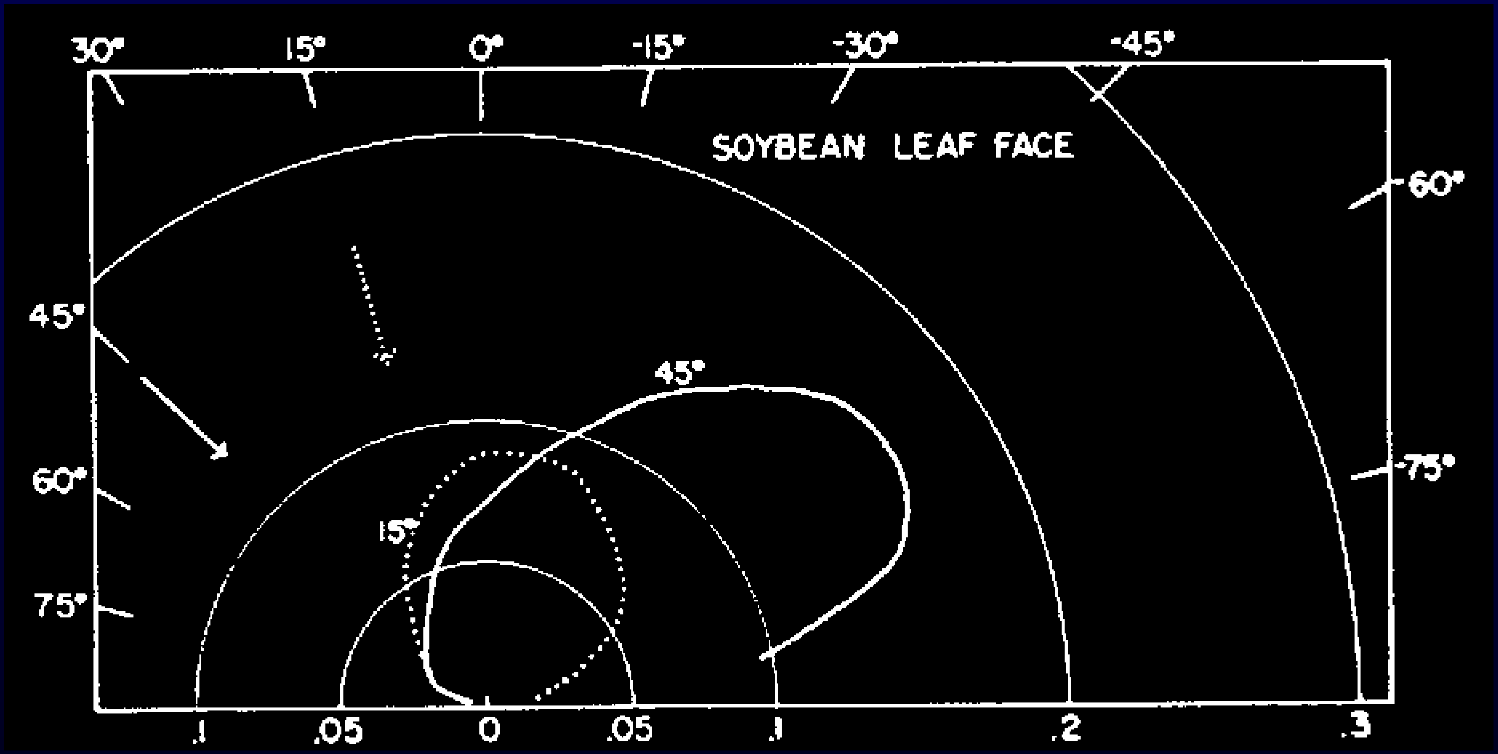
- Measurements are usually limited to a few incidence and collection geometries

Reflectance and Transmittance Measurement Geometries



- BRDF measurements are usually limited to a few cases

BRDF Data for a Soybean Leaf

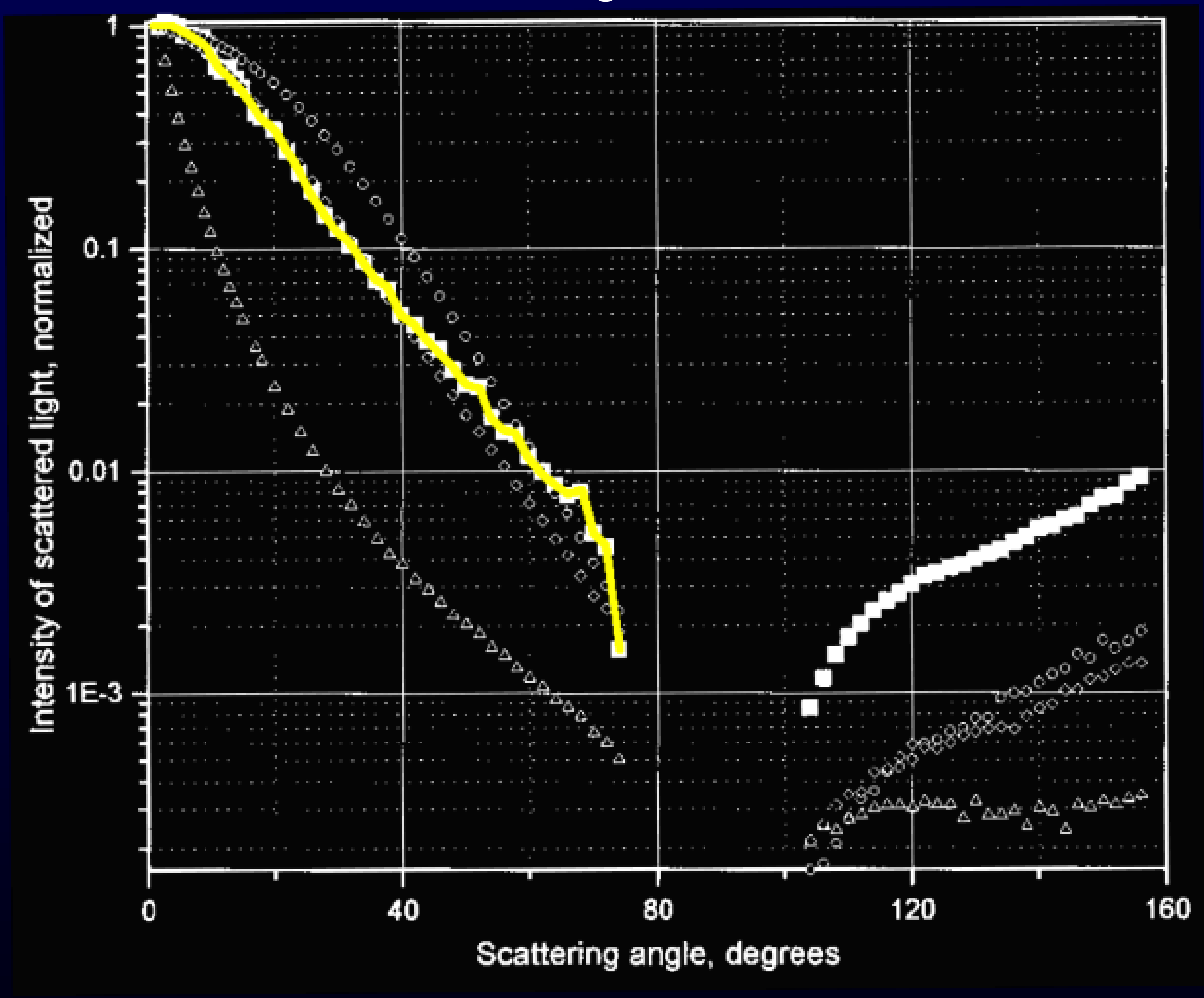


(Woolley, Plant Physiology 1971)

- Often, the following pieces of measurement related information are omitted from publications:
  - angle of incidence
  - collection geometry
  - spectral resolution (for reflectance and transmittance)
  - wavelength of interest (for scattering measurements)
  - spectral characteristics of the light source

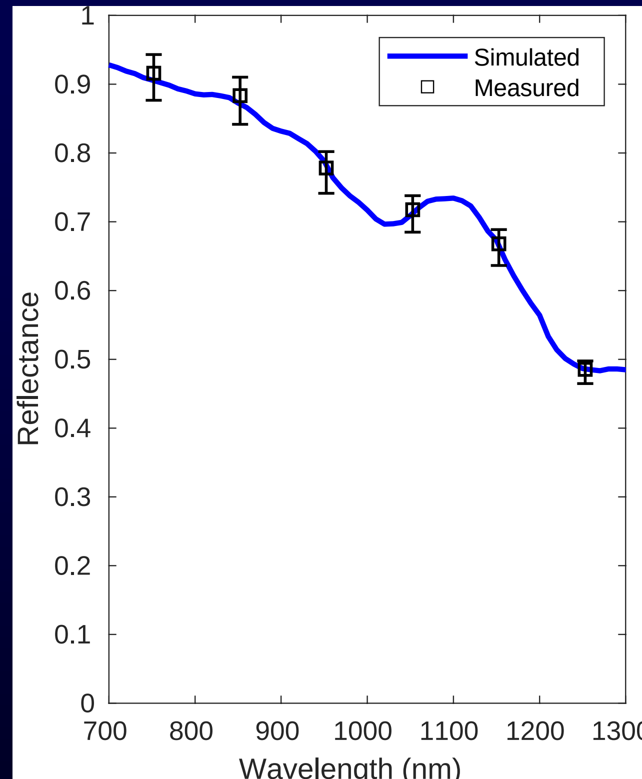
- Measured data is rarely readily available electronically

Blood Scattering Data at 613 nm



(Yaroslavsky *et al.*, Journal of Biomedical Optics 1999)

➢ How about data acquired remotely?



Measured data provided by NASA-JPL AVIRIS-NG
(Airborne Visible/Infrared Image Spectrometer)
India Campaign over Himalayan Mountains - 2016

➢ How about data acquired remotely?

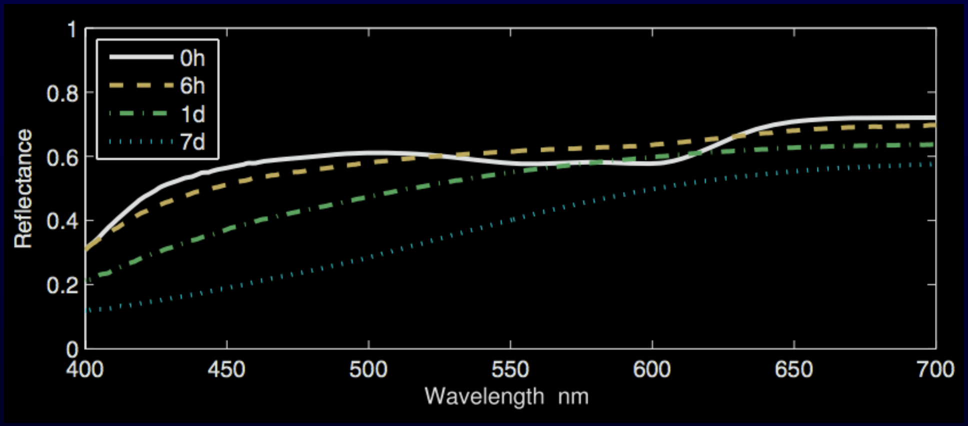
- Similar lack of characterization data

- Additional aspects to consider:
  - "image cubes" are captured during flight paths
    - ❖ each pixel is associated with hyperspectral data
  - terrain geometry
  - atmospheric conditions

➢ How about getting our own data?

- Benefits:
  - controlled experimental conditions (*e.g.*, light position and intensity)
  - wider scope of contributions (*e.g.*, measured spectral datasets)

Newsprint Yellowing (Fading)



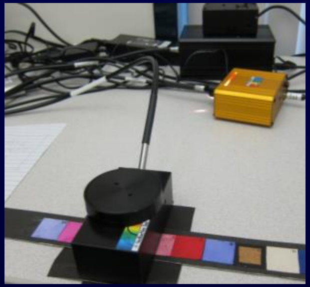
(Kimmel *et al.*, ACM TOG 2013)

How about getting our own data?

- Needs:
  - equipment (accessibility and cost constraints)
  - space and time (set up, calibration …)







- Feasibility:
  - ethical and health-related issues
  - recruitment of “volunteers”

Schedule

- ✓ Introduction
- ✓ Biophysical Background
- ✓ Drawing Board
- ✓ Data Availability and Quality

Break

- ❑ Design Issues
- ❑ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

Schedule

- ✓ Introduction
- ✓ Biophysical Background
- ✓ Drawing Board
- ✓ Data Availability and Quality

Break

- ❑ Design Issues
- ❑ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

Design Issues

- Level of Abstraction
- Simplifying Assumptions
- Generalizations
- Iterative Refinement
- Algorithmic Evolution

Level of Abstraction

"From an optical point of view, a leaf is more complex than a lake or a sea, indeed, a more complex object is difficult to imagine!

The possible combinations of optical phenomena are astronomical!"

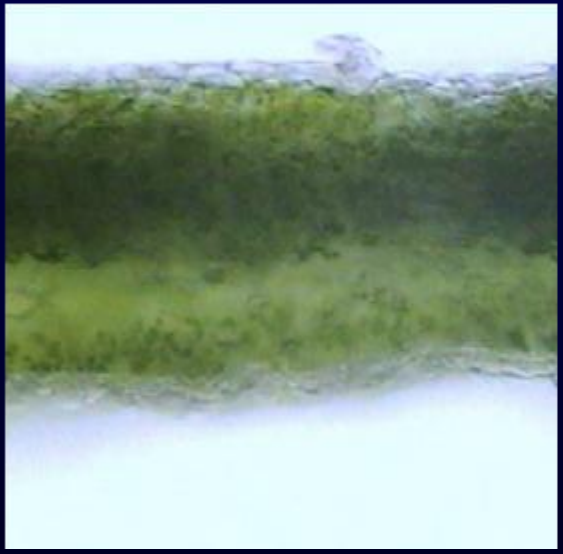
M.G.J. Minnaert (1974)
Light and Color in the Outdoors

➢ How can we represent real materials?

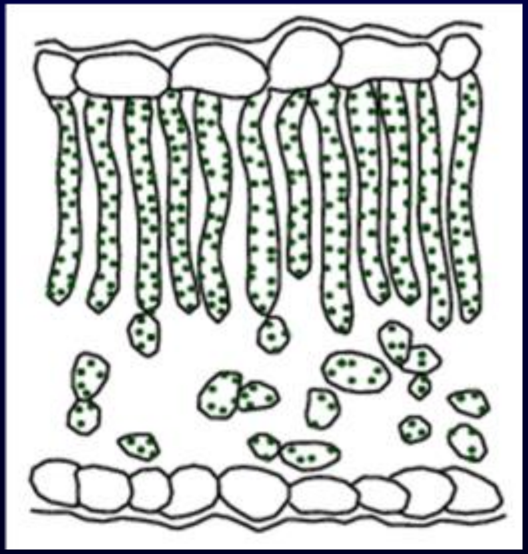
- Example: plant leaves

Bifacial Leaves

Cross-Section (OM)

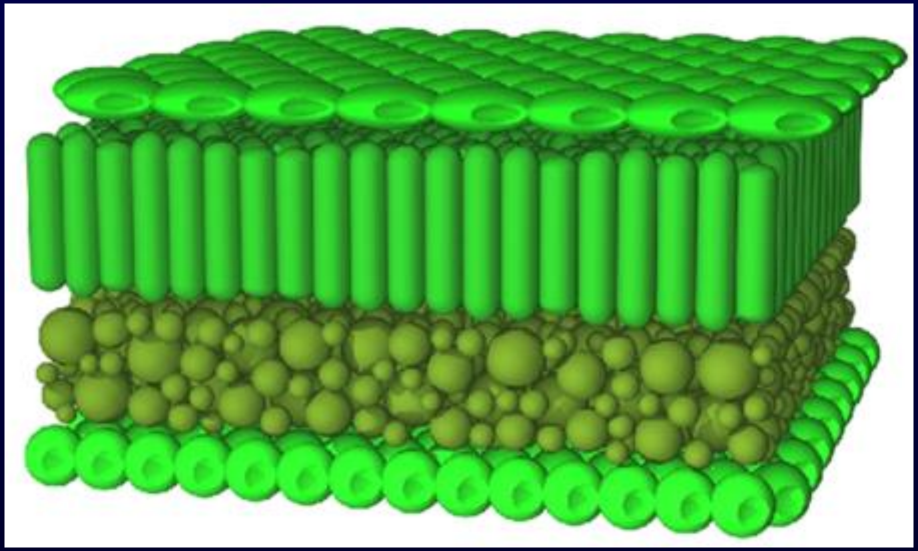


Cross-Section (sketch)



- How about considering the full material description?

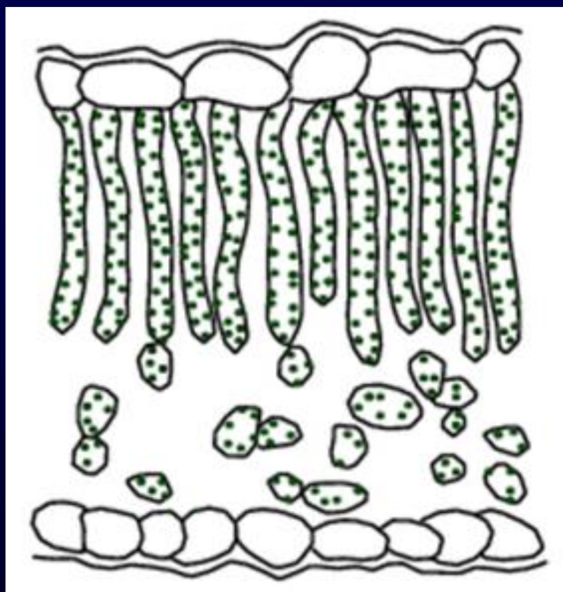
3D Representation Used by the Raytran Model



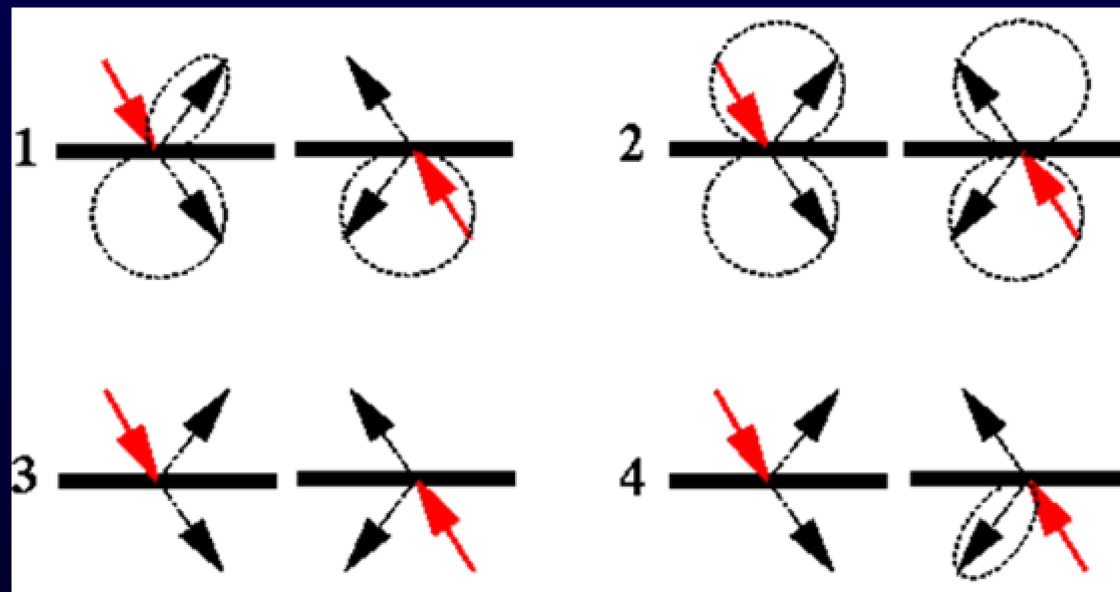
(Govaerts *et al.*, Applied Optics, 1996)

- Alternatively, we can represent the material using “layers”

Cross-Section

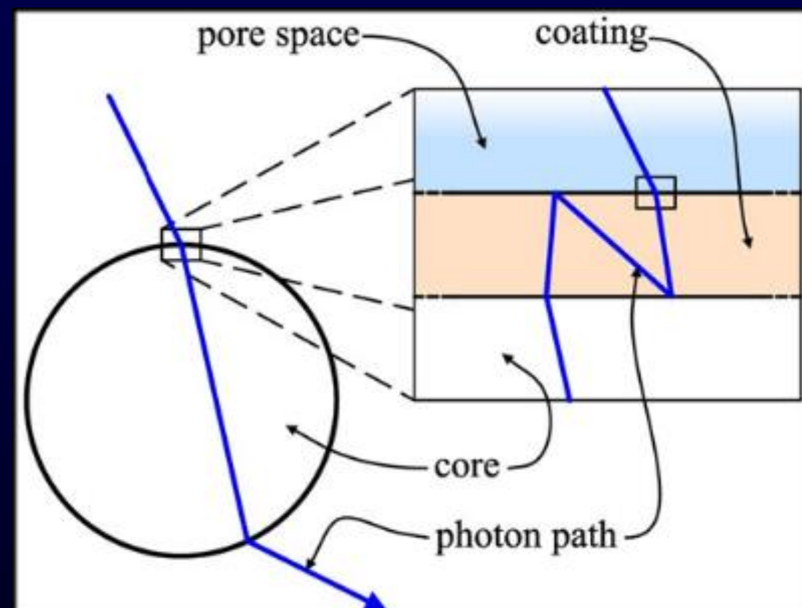


Layered ABM Model for Plant Leaves



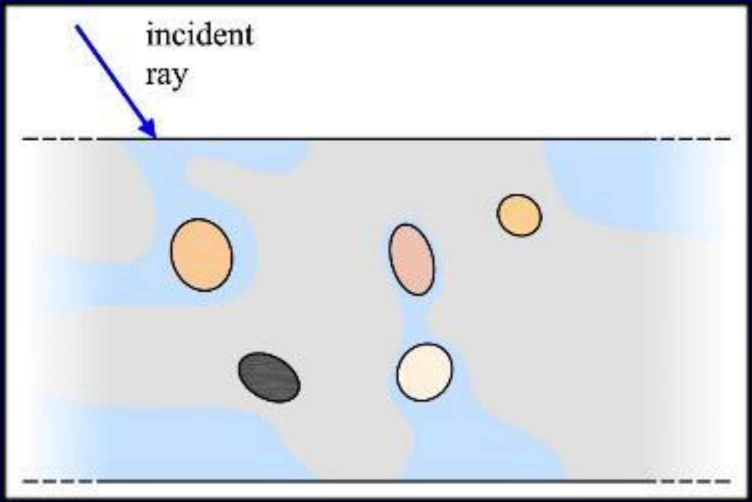
- How about combining both approaches?

  - SPLITS model considers the light interactions with individual sand grains and within each layer of a sand grain coating

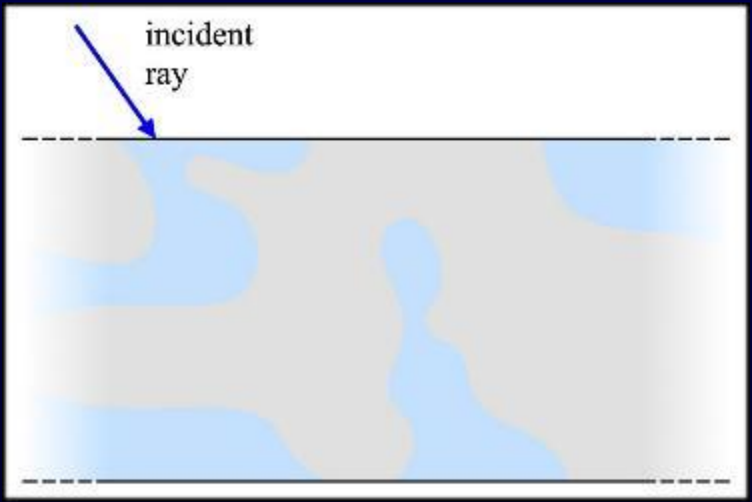


  - SPLITS generates sand grains on the fly during the simulations

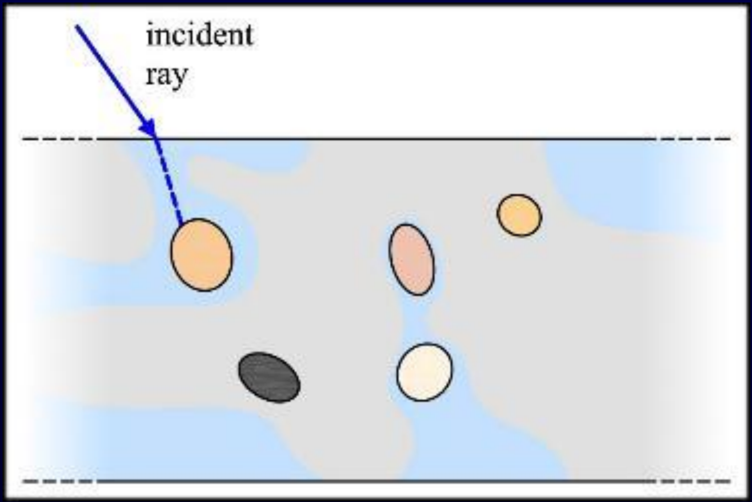
Ray Tracing



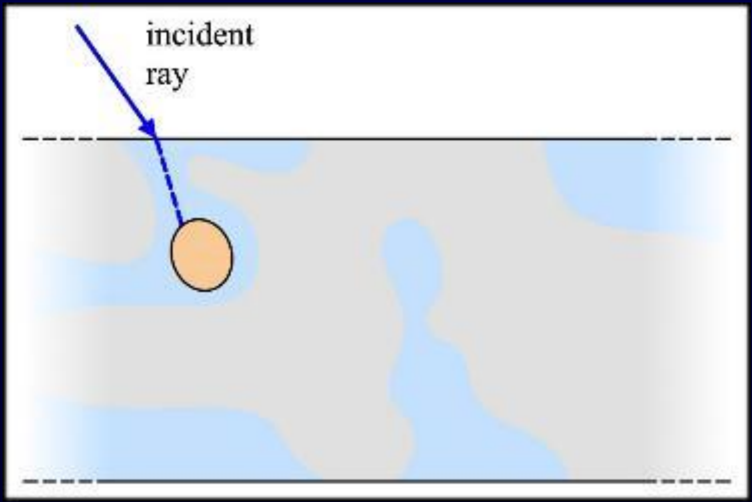
SPLITS



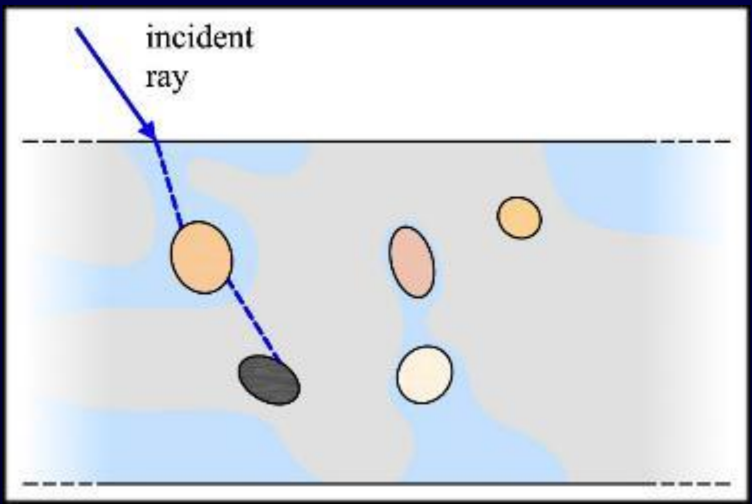
Ray Tracing



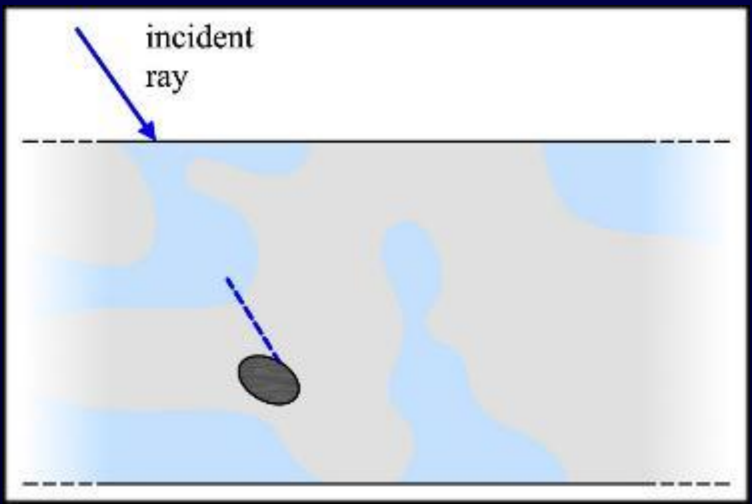
SPLITS



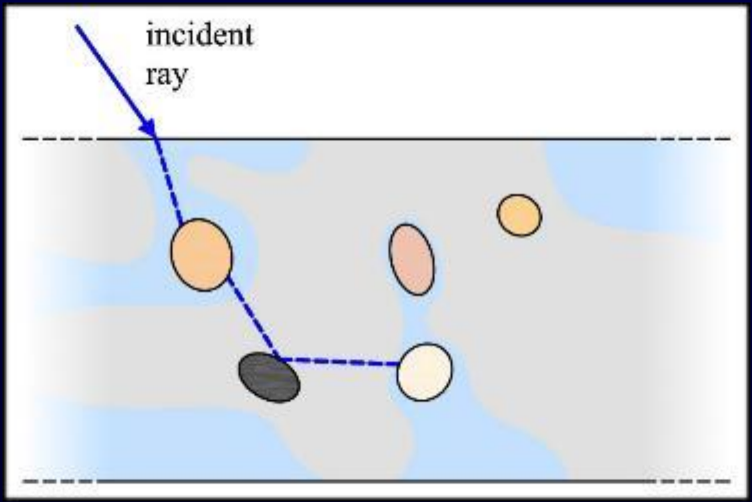
Ray Tracing



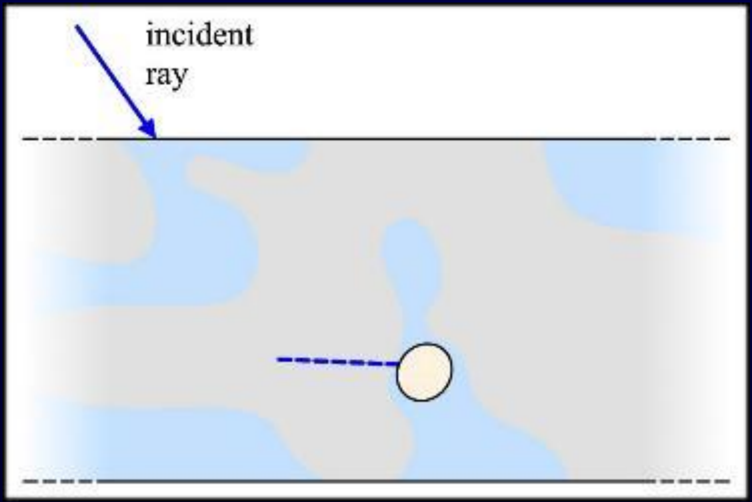
SPLITS



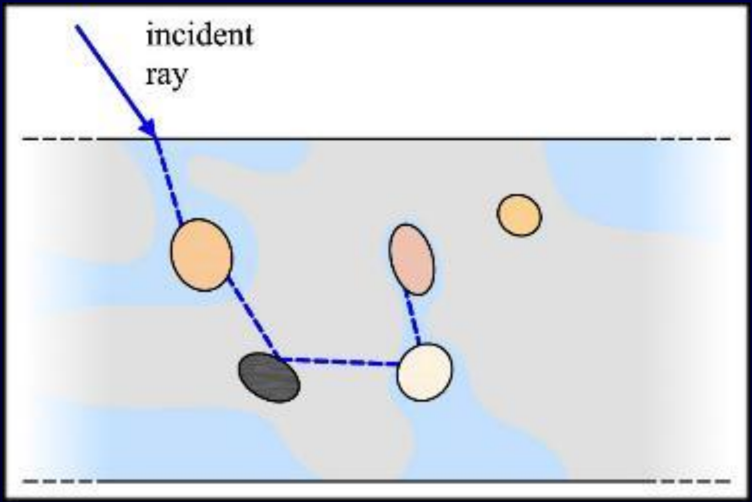
Ray Tracing



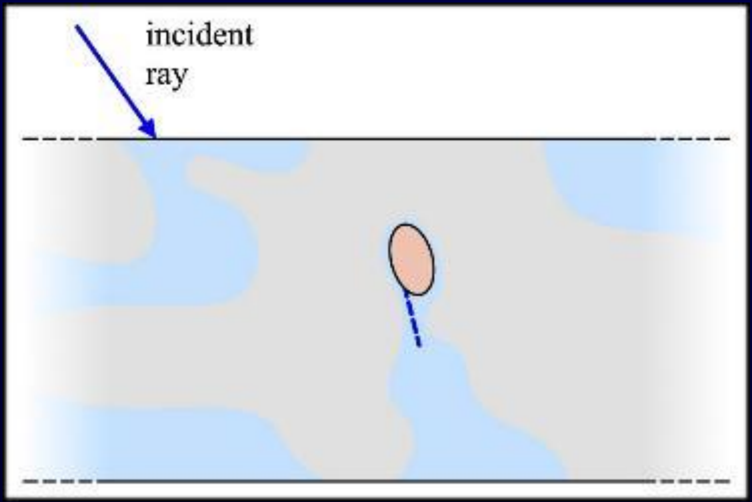
SPLITS



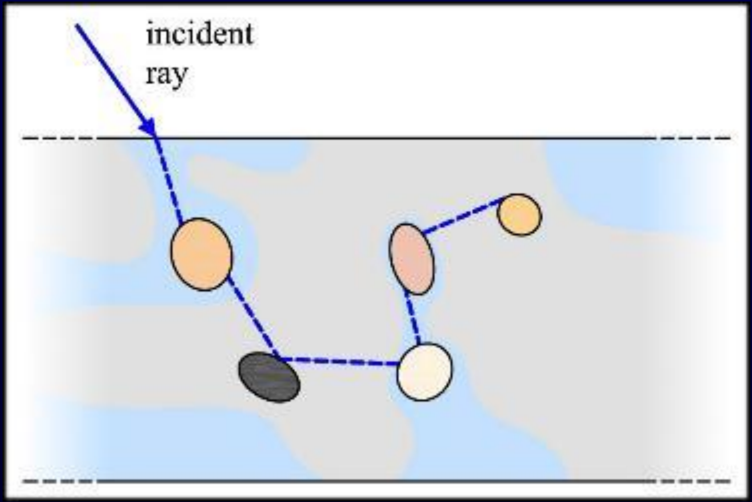
Ray Tracing



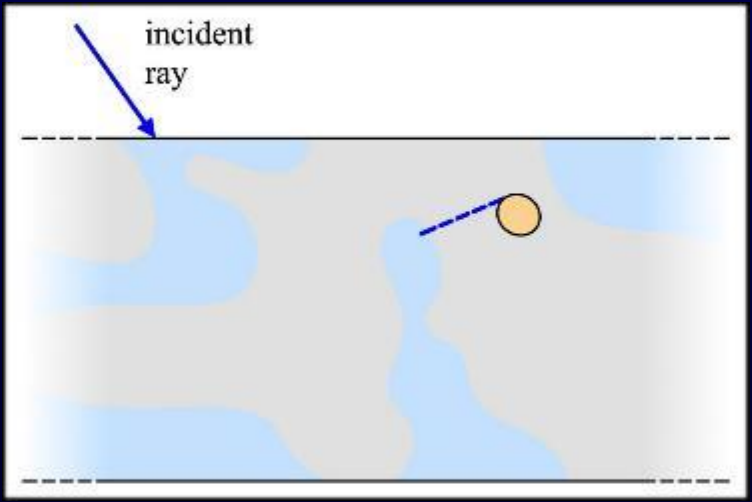
SPLITS



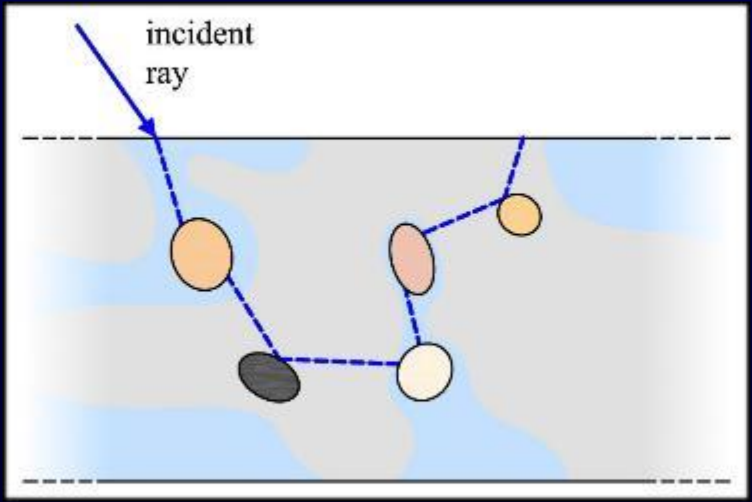
Ray Tracing



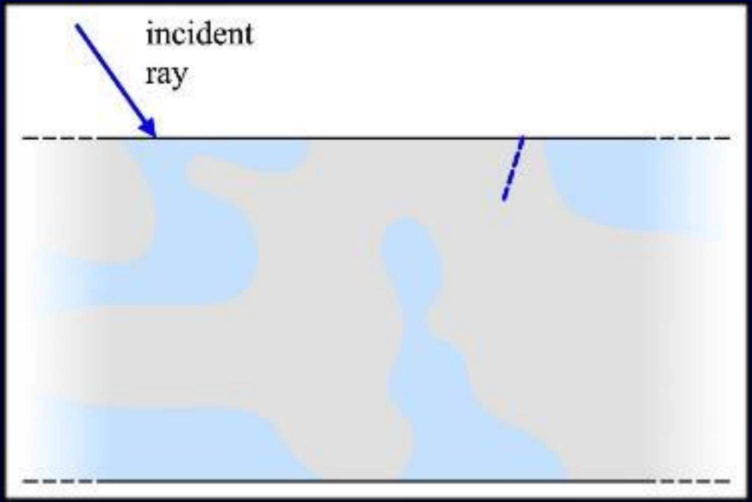
SPLITS



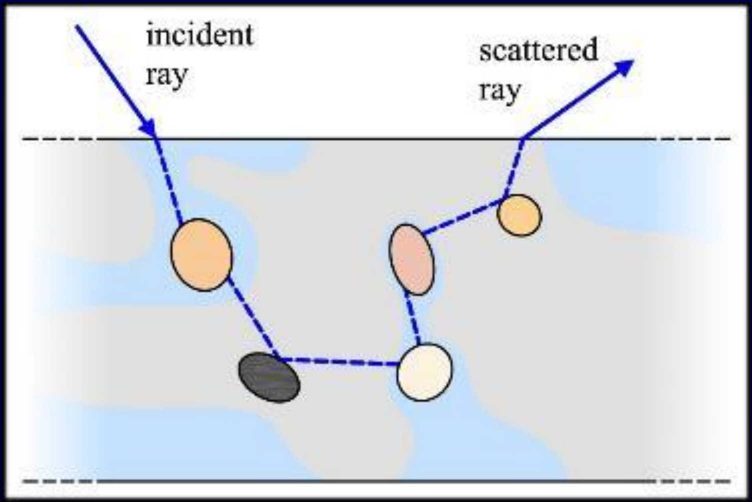
Ray Tracing



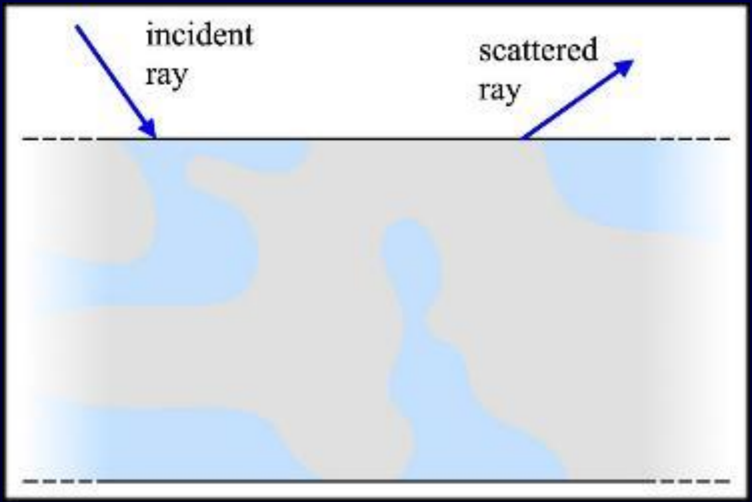
SPLITS



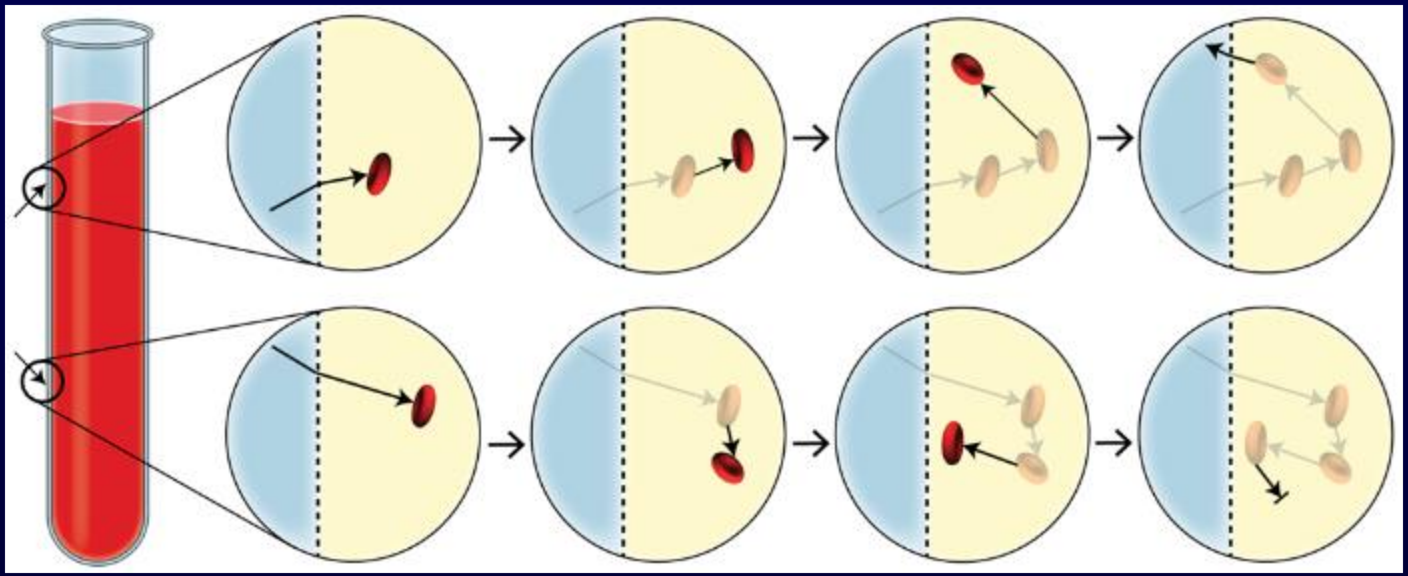
Ray Tracing

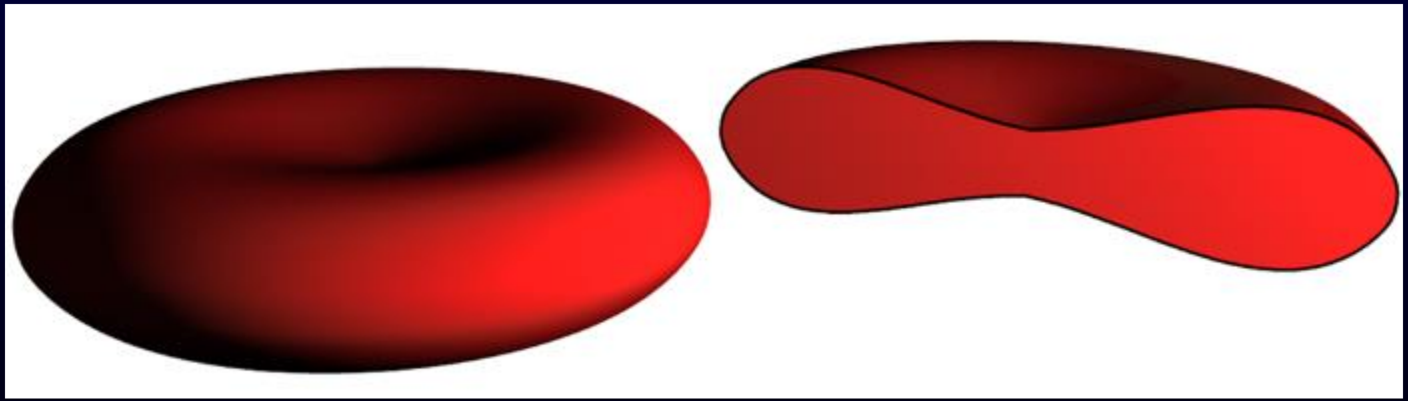


SPLITS



Examples of ray (light) propagation/attenuation processes taken into account by the CLBlood model using the “SPLITS approach”





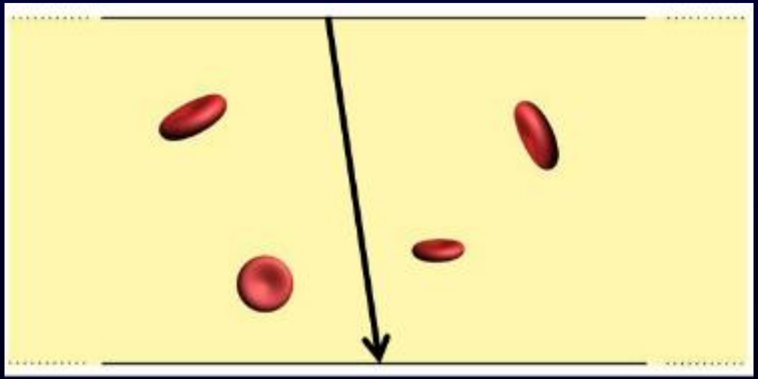
- Summary
  - There are different ways to represent the materials
  - No representation is superior in all cases
  - The best representation for a given application will depend on:
    - data constraints
    - simulation approach
    - fidelity requirements
    - performance requirements

Simplifying Assumptions

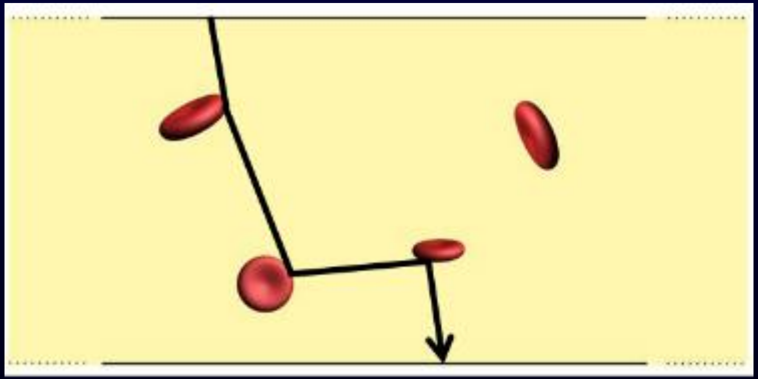
➢ “Material is homogeneous”

- Counter-example: optical behaviour of whole blood differs from that of a hemoglobin solution (with the same pigment concentration) due to sieve and detour effects

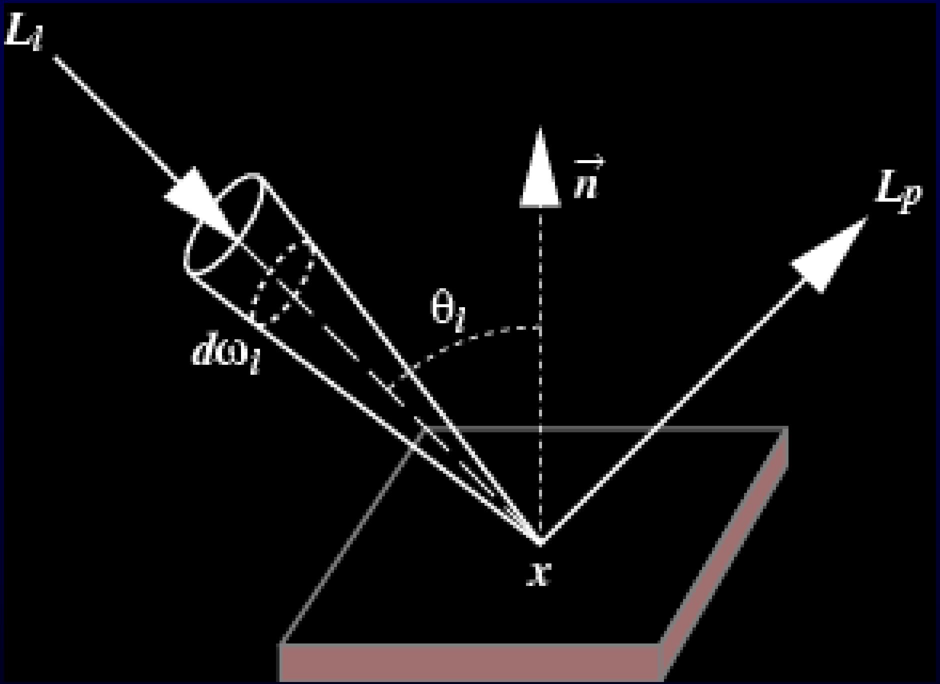
Sieve Effect



Detour Effect



- “Material is isotropic”



- Counter-example: plant leaves with parallel venation systems

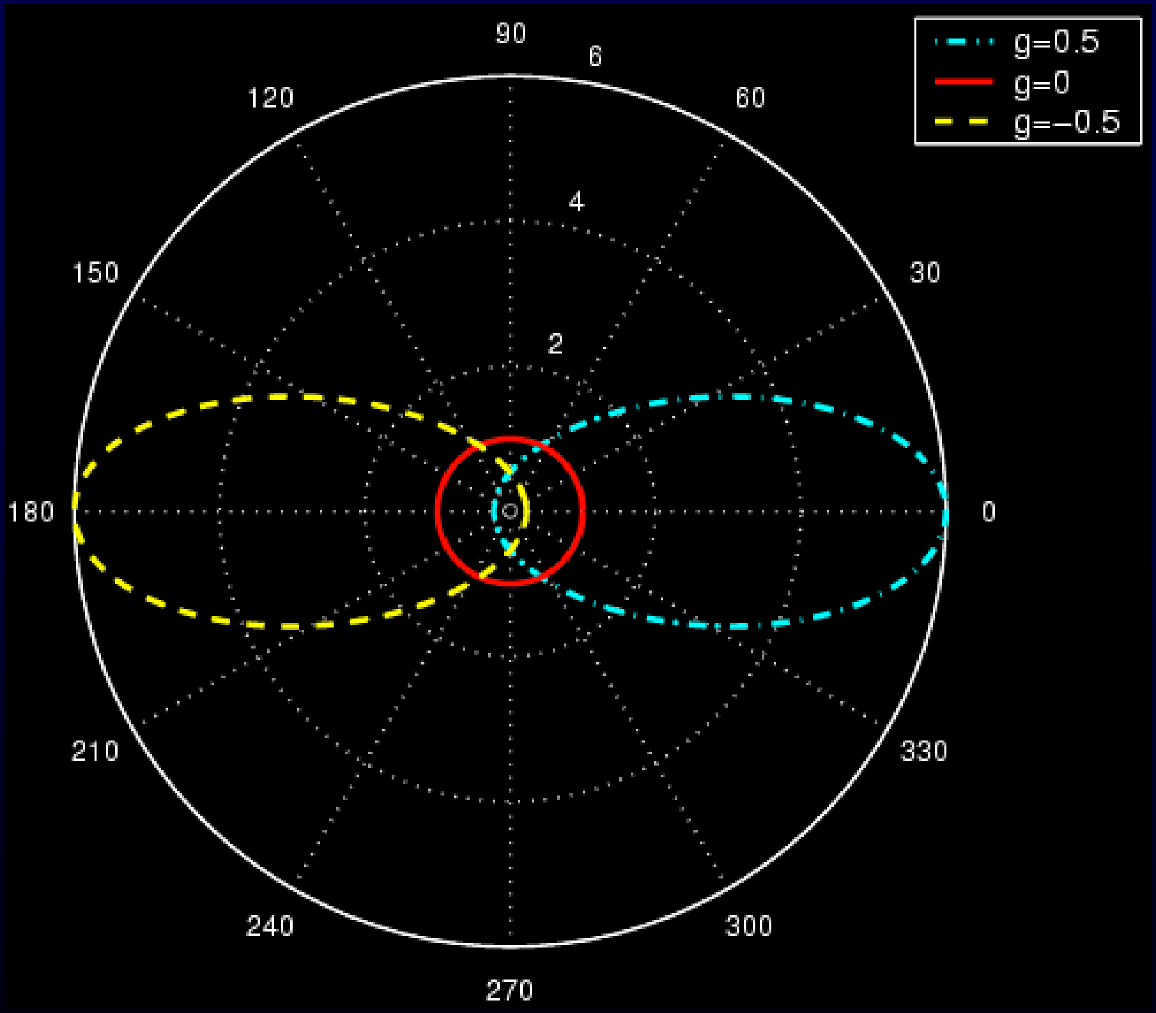
Generalizations

- Use of phase functions to approximate bulk scattering

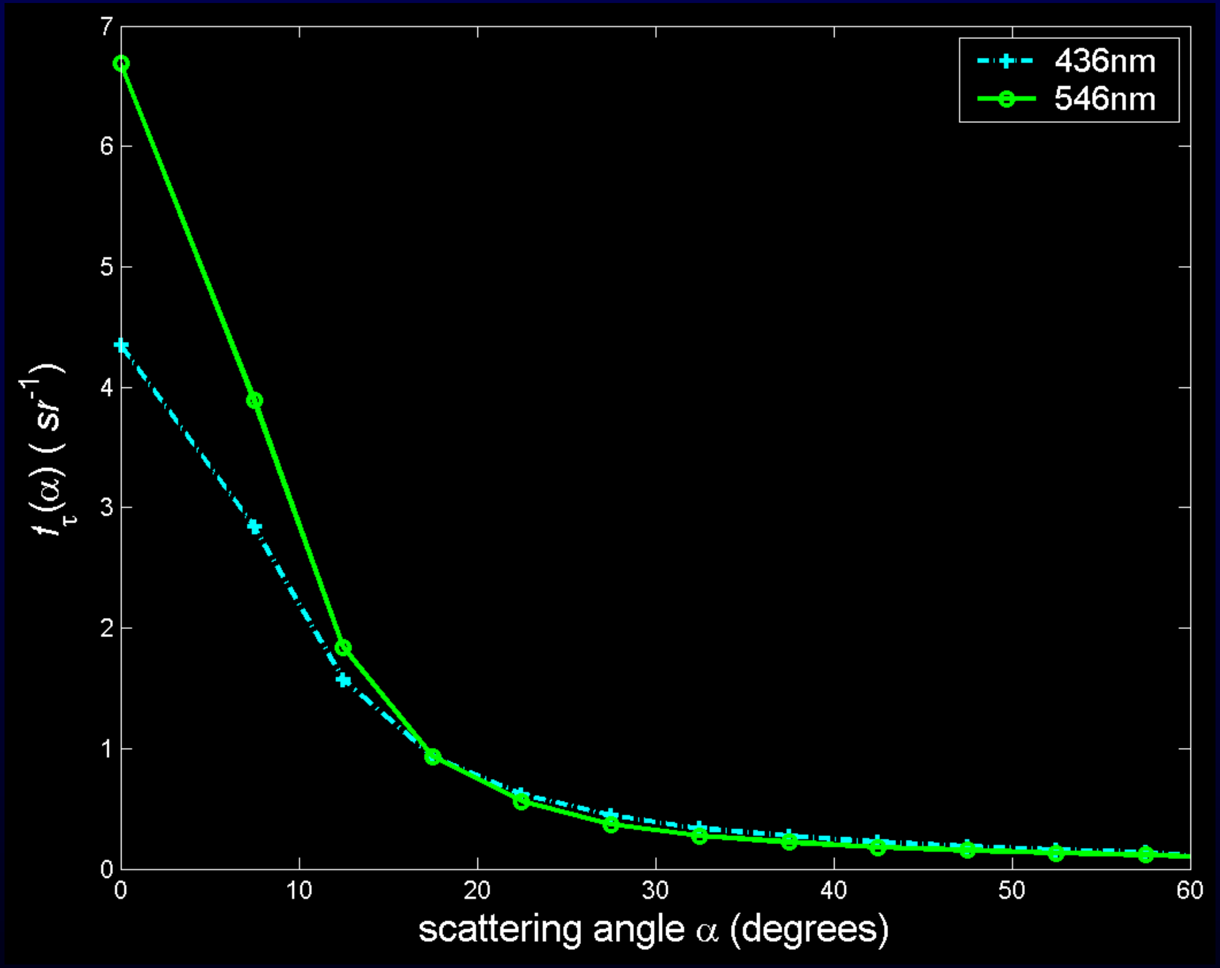
  - Bruls and van der Leun (1984) suggested that their measured skin (subsurface) scattering data (at 254nm, 302nm, 365nm, 436nm and 546nm) could be approximated by a phase function tabulated by van de Hulst …

… the Henyey-Greenstein phase function (HGPF)

$$\Gamma_{HG}(g,\alpha) = \frac{1-g^2}{(1+g^2-2g\cos\alpha)^{\frac{3}{2}}}$$

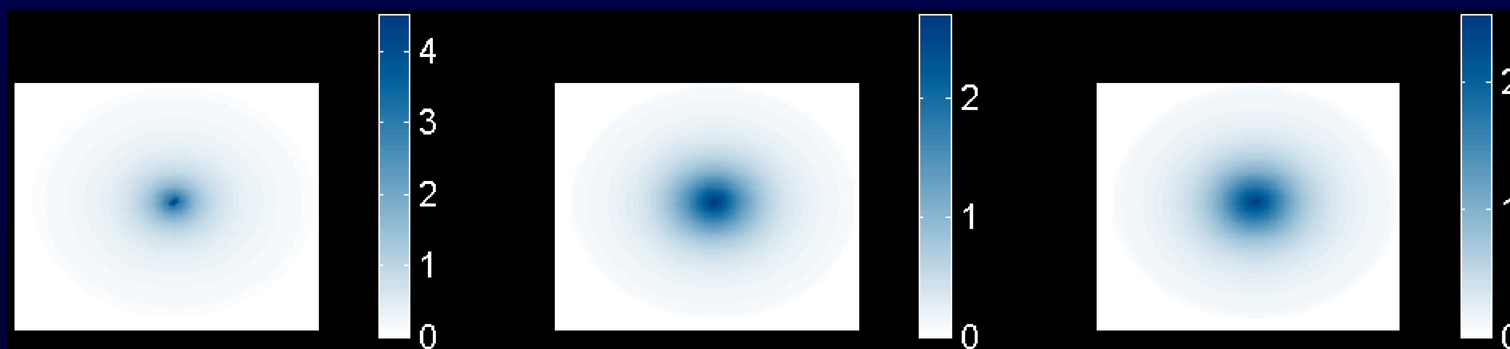


BTDF Values for the Epidermis



Comparison of Measured (at 436nm) and Modeled Data for Epidermis

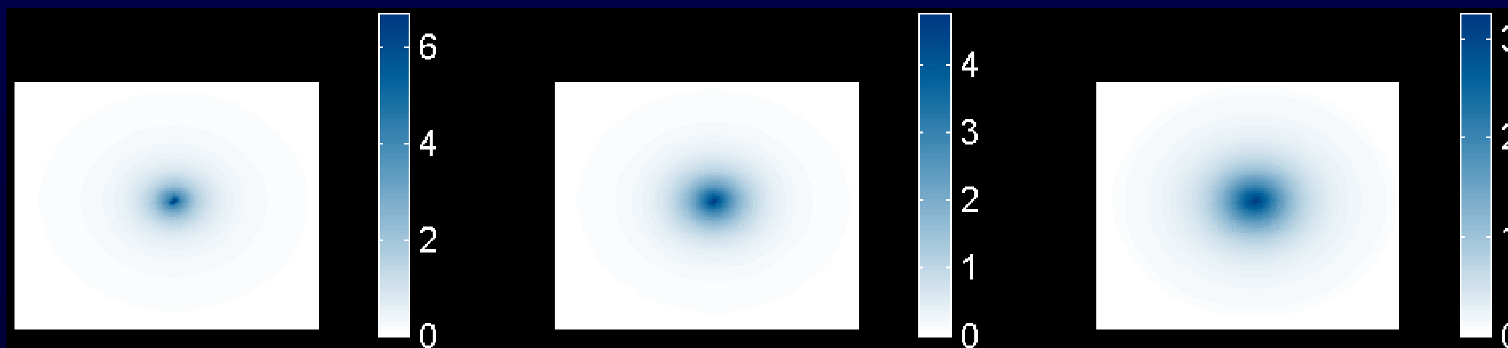
Measured | HGPF, *g*=0.761 | HGPF, *g*=0.748



data | *RMS* error | least squares

Comparison of Measured (at 546nm) and Modeled Data for Epidermis

Measured | HGPF, g=0.821 | HGPF, g=0.781



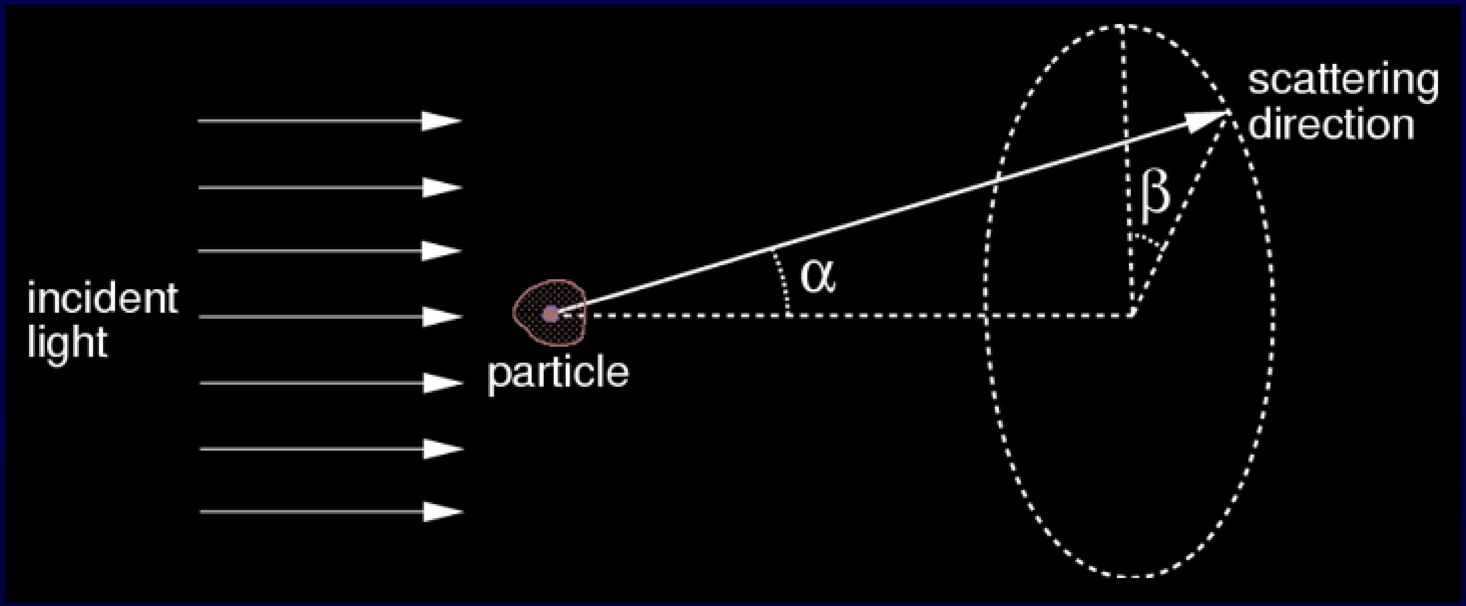
data | *RMS* error | least squares

- Prahl's Monte Carlo based model (1988)
  - aim: light transport in tissue during laser radiation
  - computes photon trajectories using a warping function derived (Witt 1977) from the HGPF

$$(\alpha, \beta) = \left(\arccos \left[\frac{1}{2g} \left\{ 1 + g^2 - \left[\frac{1 - g^2}{1 - g + 2g\xi_1} \right]^2 \right\} \right], 2\pi\xi_2 \right)$$

where:

ξ_1 and ξ_2 = uniformly distributed random numbers $\in [0, 1]$.



$$(\alpha, \beta) = \left(\arccos \left[\frac{1}{2g} \left\{ 1 + g^2 - \left[\frac{1 - g^2}{1 - g + 2g\xi_1} \right]^2 \right\} \right], 2\pi\xi_2 \right)$$

where:

ξ_1 and ξ_2 = uniformly distributed random numbers $\in [0, 1]$.

- Pros and cons of applying the HGPF in the simulation of light scattering by different materials:
  - relatively easy to use
  - it makes the papers look “cool”
  - it is not based on a mechanistic theory of scattering
  - it does not have a biophysical basis
  - it provides a fidelity/cost ratio lower than data-driven approaches

- In the absence of comprehensive measured data, one can resort to warping functions with a higher fidelity/cost ratio

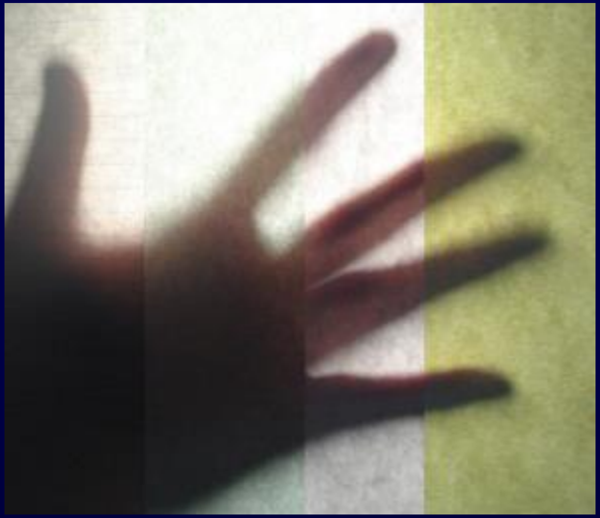
- Example: warping function derived from an exponentiated (*n*) cosine (EC) distribution

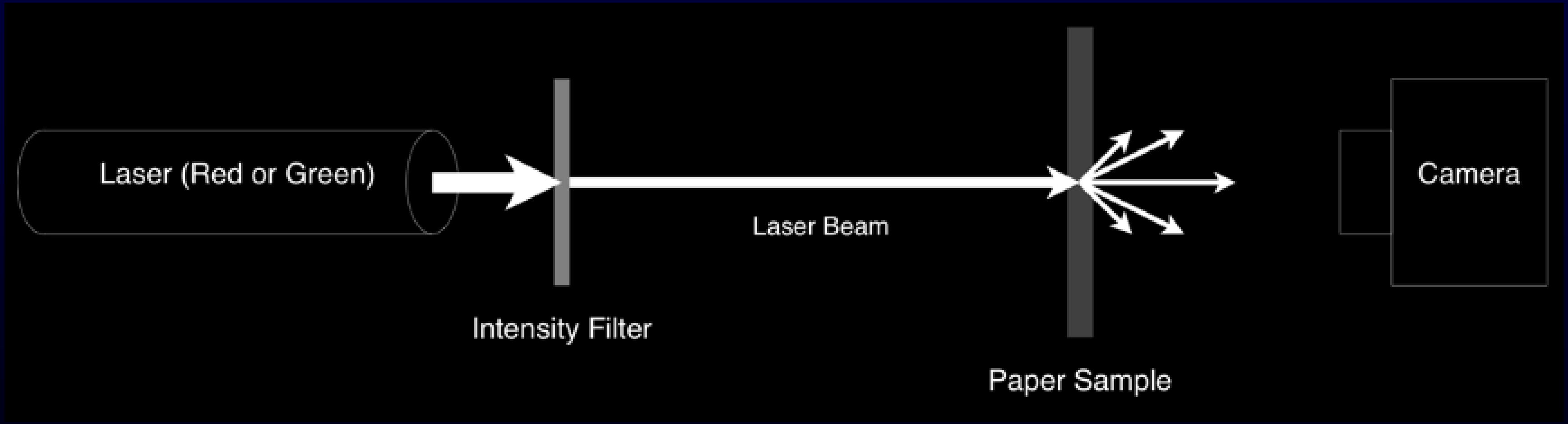
$$(\alpha, \beta) = (arccos(1 - \xi_1)^{\frac{1}{n+1}}, 2\pi\xi_2)$$

where:

ξ_1 and ξ_2 = uniformly distributed random numbers $\in [0, 1]$.

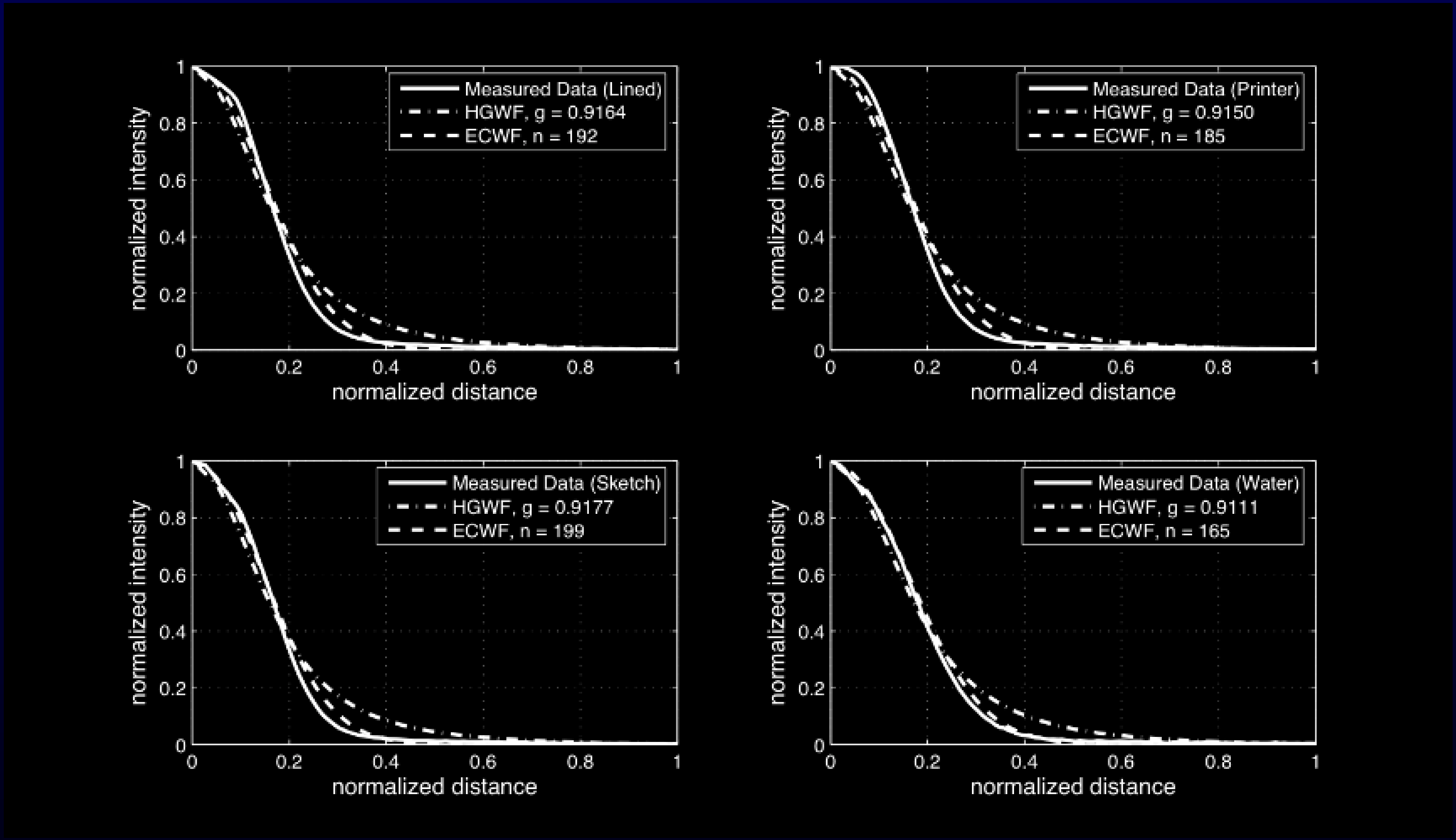
- Experiments involving different types of paper





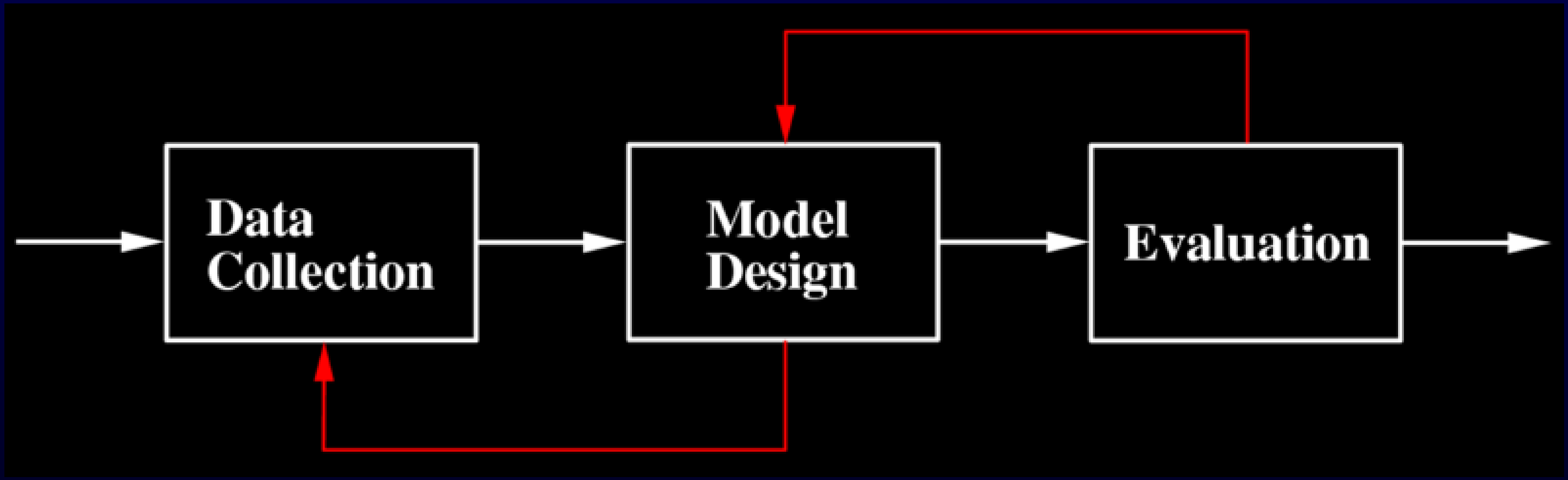
(Chen and Baranoski, Optics Express 2008)

Comparison of Measured (at 543nm) and Simulated Scattering Data for Paper



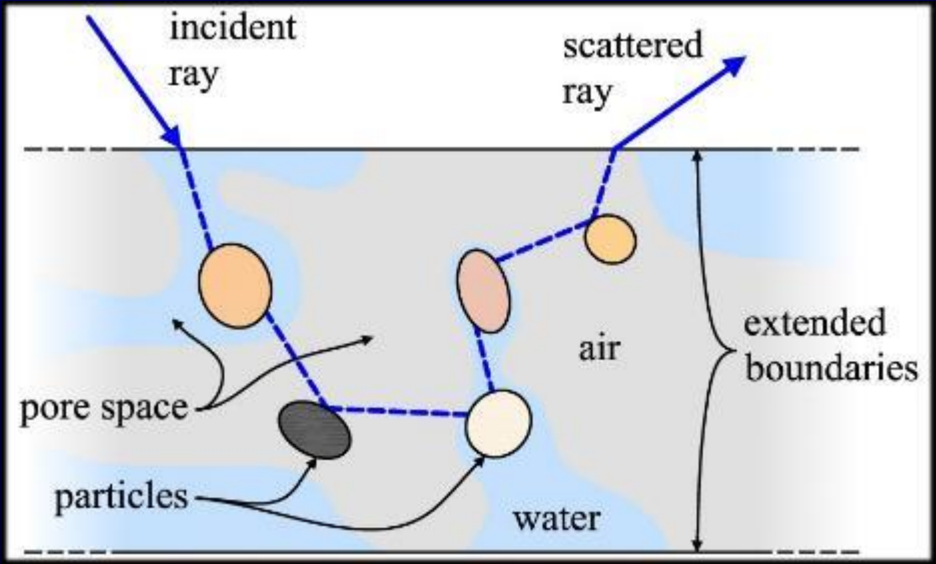
Iterative Refinement

- Recall that a model development framework is seldom linear



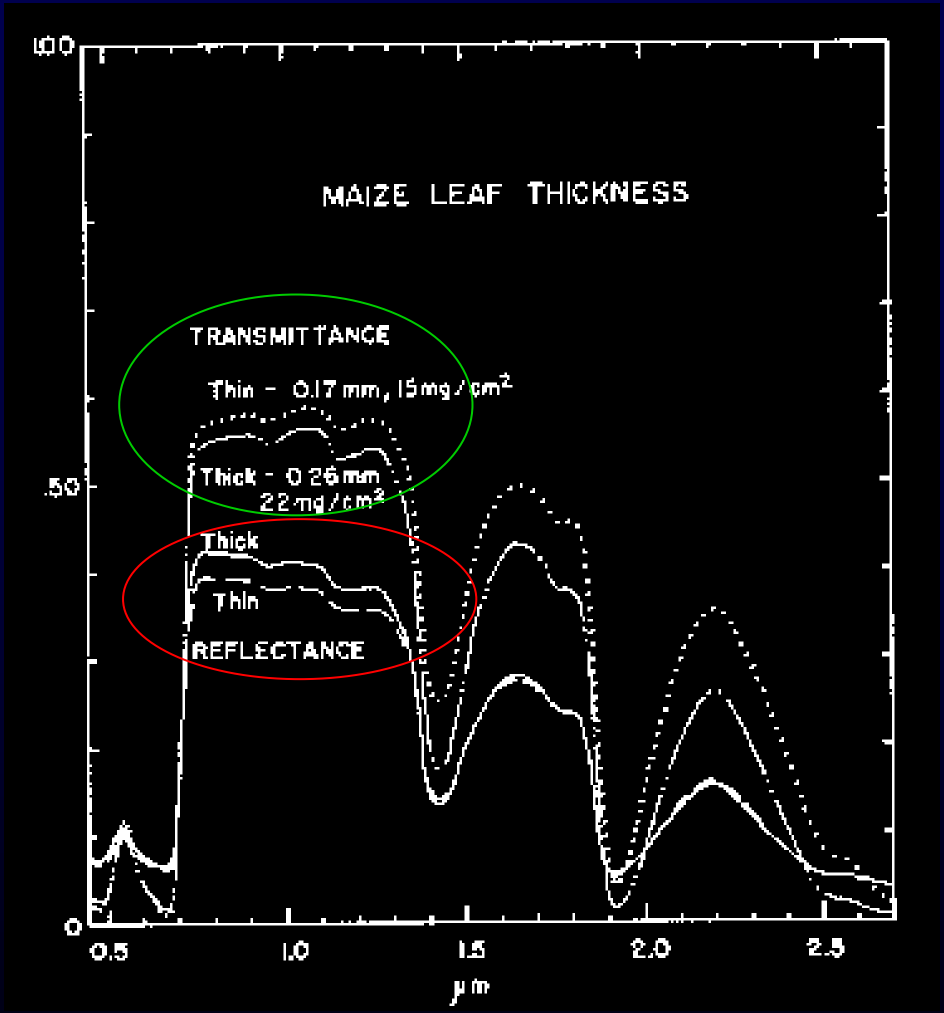
- Key insights can be obtained through *in situ* observations …

  - Example: SPLITS simulations



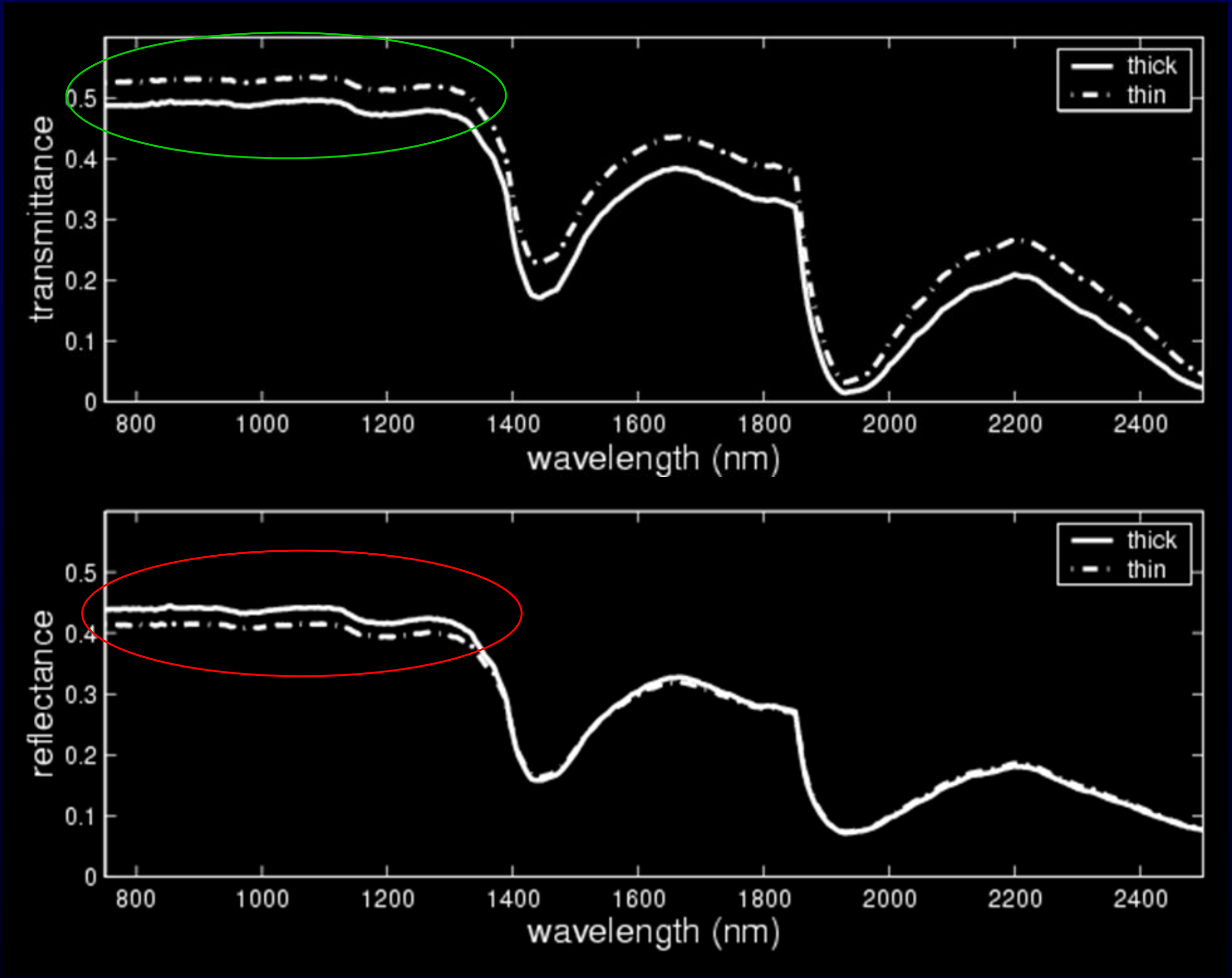
➢ … and qualitative comparisons with experimental data

- Example:



(Woolley, Plant Physiology 1971)

Modeled (ABM-U) Corn Spectral Curves



➢ What if the materials to be modeled are not fully understood?

- Example: composition of Martian regolith

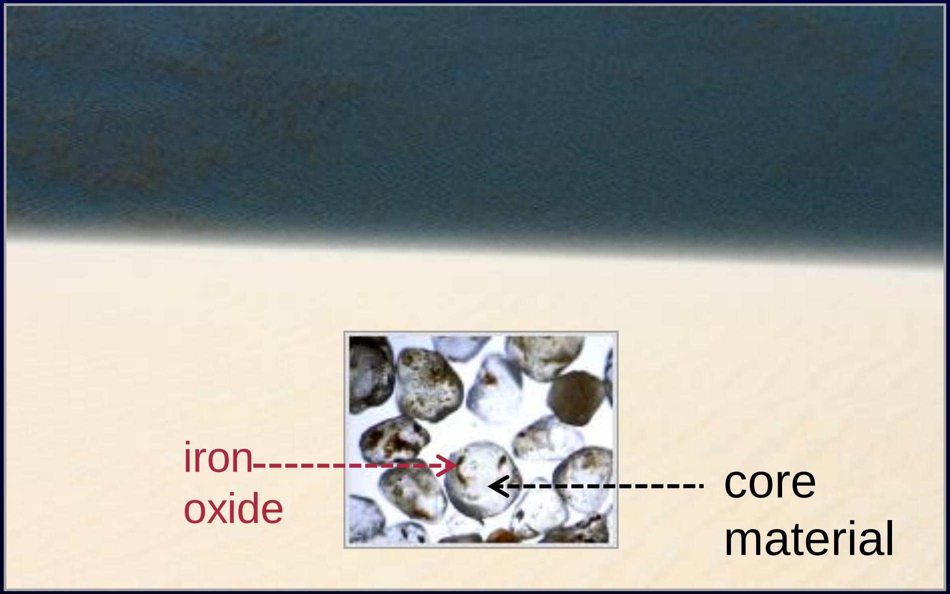
“Spot the difference: the Atacama desert in Chile (left) shares many features with the surface of Mars (right)”

(“Secrets of Martian Soil” by C. Wu, Nature 2007)

➢ What if the materials to be modeled are not fully understood?

- Example: composition of Martian regolith

However, while the core materials of terrestrial sand-textured soils can be clearly identified …

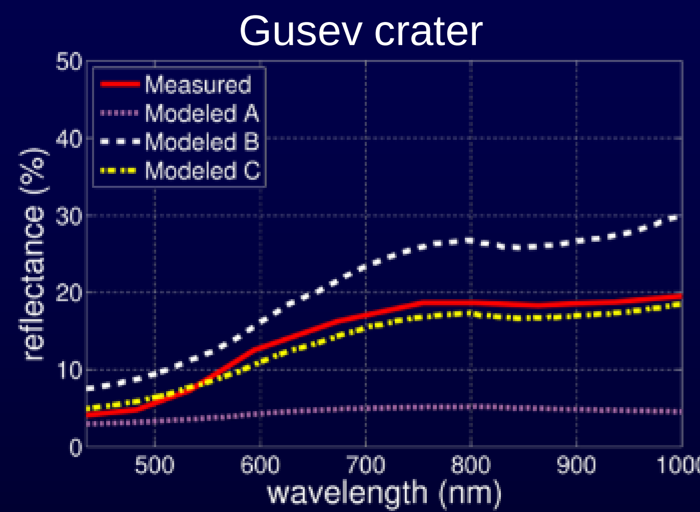


the same cannot be said about Martian regolith

➢ What if the materials to be modeled are not fully understood?

- Example: composition of Martian regolith

Measured data acquired by a multispectral camera on board the Spirit rover's (Bell III *et al.*, Science 2004**)**



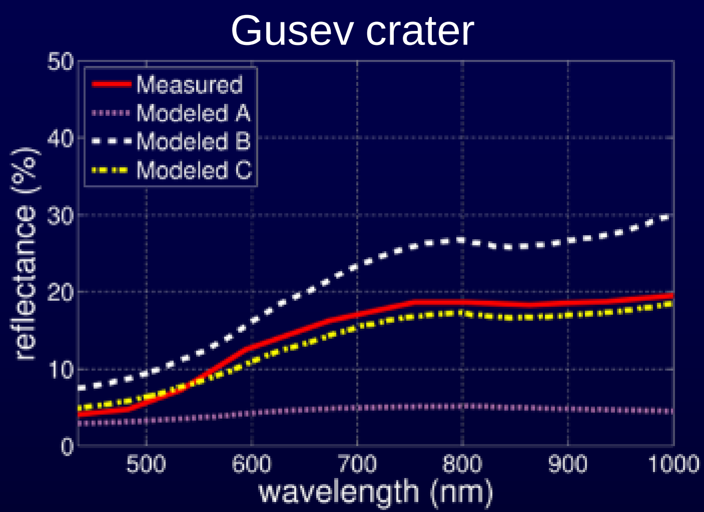
Modeled A: basalt as the core of mixed, coated and pure grains

Modeled B: quartz as the core of mixed, coated and pure grains

➢ What if the materials to be modeled are not fully understood?

- Example: composition of Martian regolith

Bright-toned soil unveiled by the Spirit rover's faulty wheel (Squyres *et al.*, Science 2008)



Modeled A: basalt as the core of mixed, coated and pure grains

Modeled B: quartz as the core of mixed, coated and pure grains

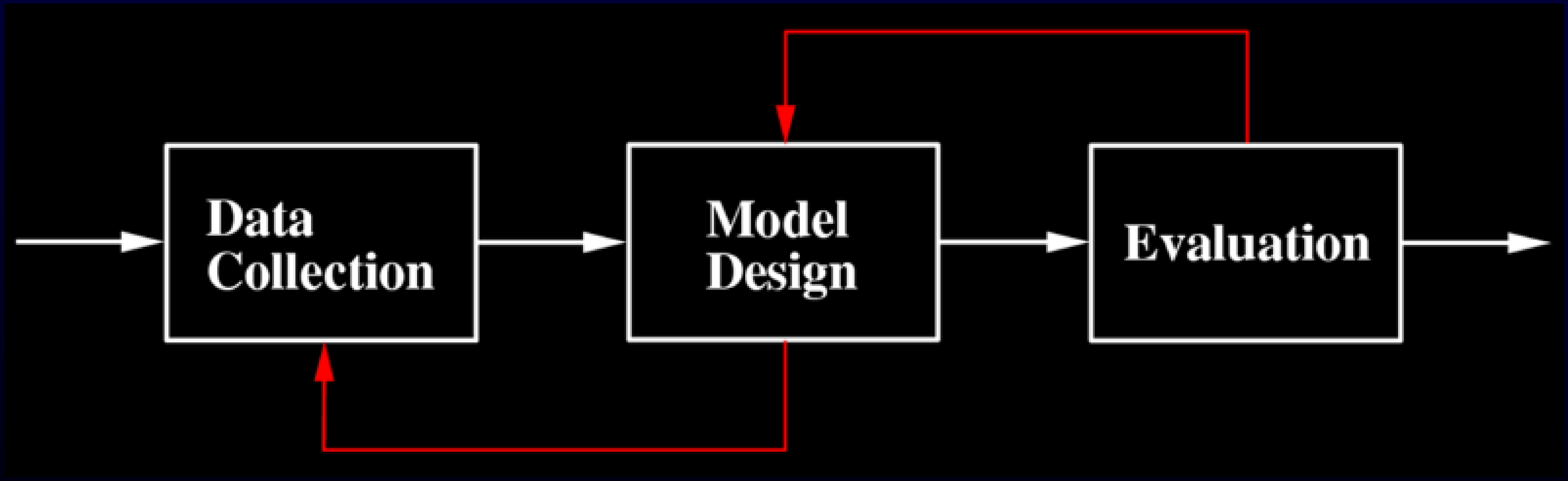
Modeled C: silica-rich basaltic compositions as the core of mixed grains and basalt as the core of coated and pure grains

(Baranoski *et al*., IEEE IGARSS 2014 & 2019, IEEE JSTARS 2015)

➢ Interaction with experimental investigation

- A model should enable the prediction of the spectral responses of a given material under various conditions

- Including those not yet experimentally tested, and thus not addressed during the model development process



“The most exciting phrase to hear in science,
the one that heralds new discoveries,
is not ‘Eureca!’ (‘I’ve found it!),
but ‘That’s funny …’”

Isaac Asimov

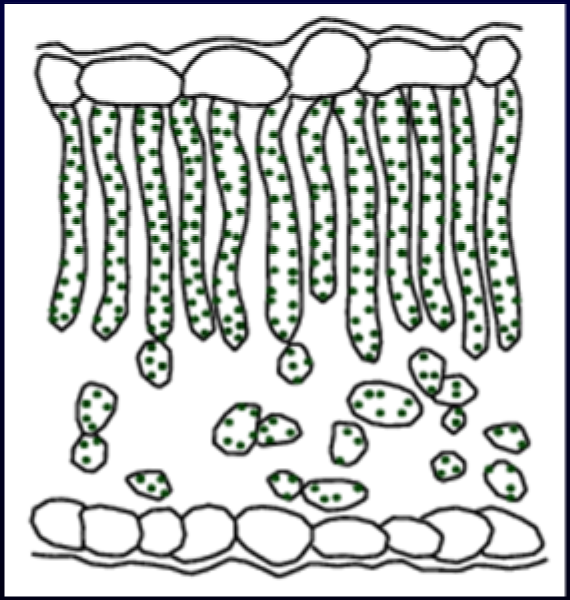
Check it out:

“The color of shock waves in photonic crystals”
(Reed *et al.*, Physical Review Letters 2003)

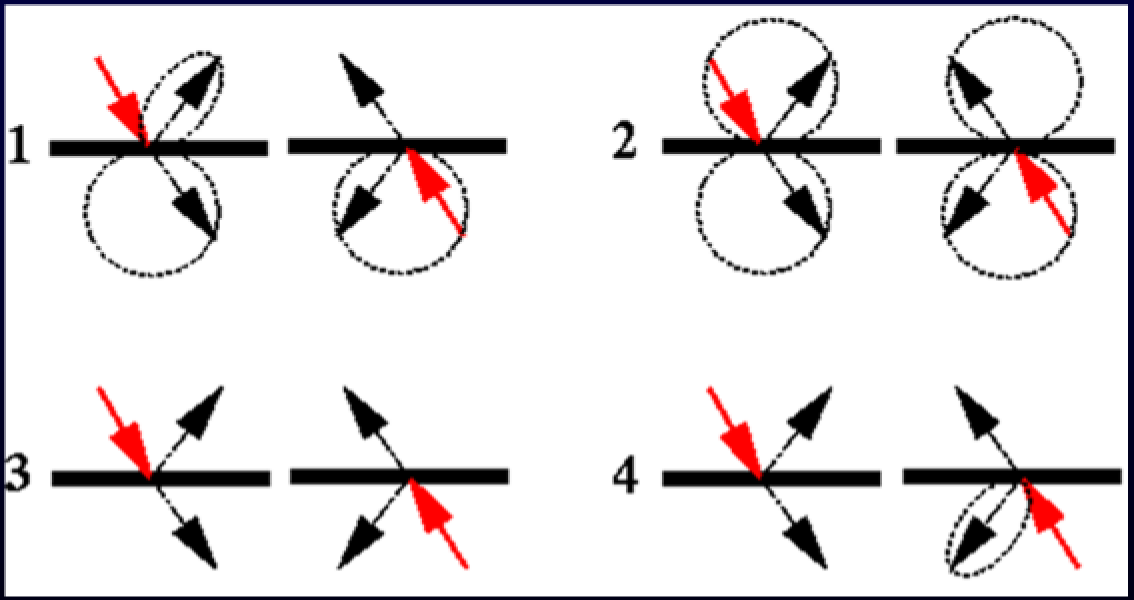
Algorithmic Evolution

- Oftentimes driven by application requirements
  - Example: recall the ABM model for (bifacial) plant leaves

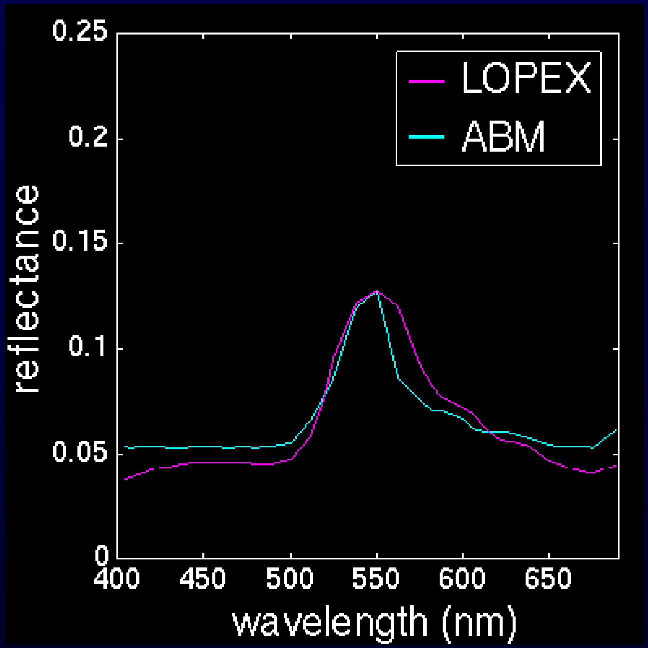
Cross-Section

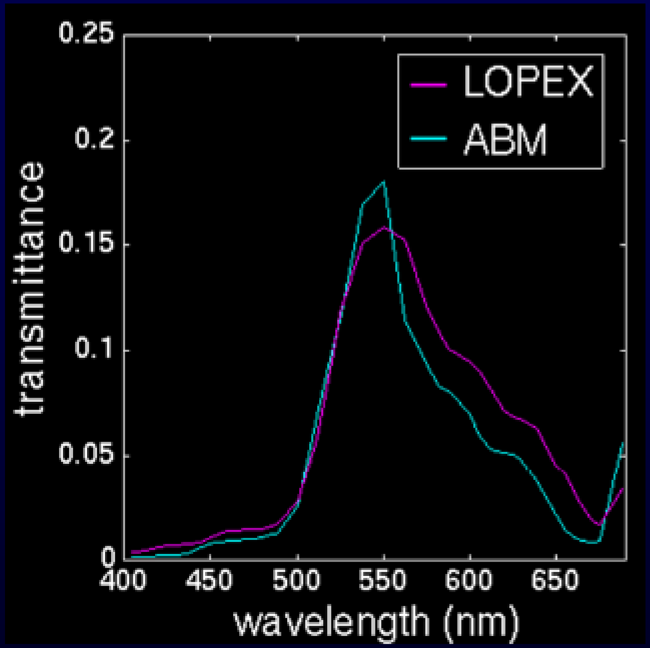


Layered ABM Model for Plant Leaves



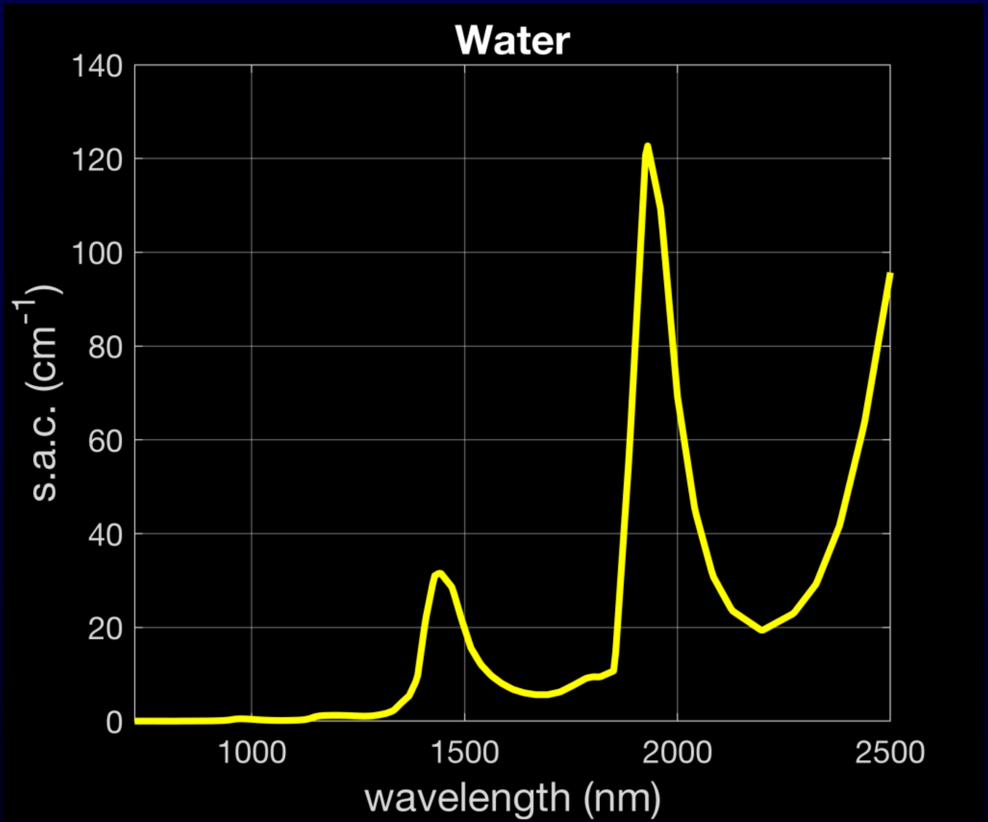
Measured (LOPEX) and Modeled (ABM) Soybean Spectral Signatures



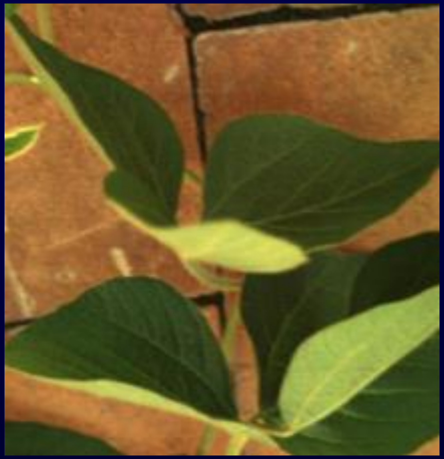


- How about spectral signatures in the infrared domain?

- What is the major absorber in this domain?

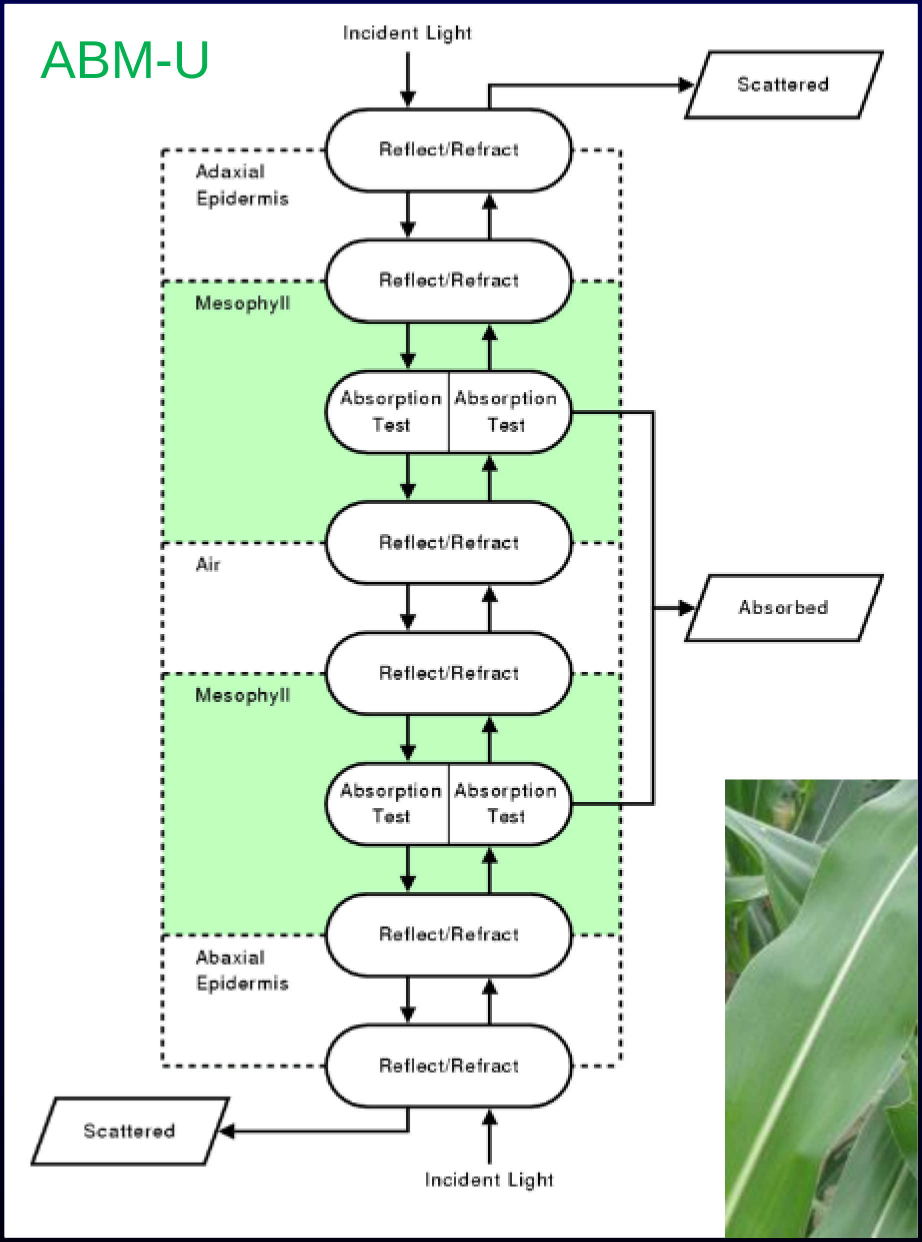


- How about structural differences between bifacial and unifacial plant leaves?



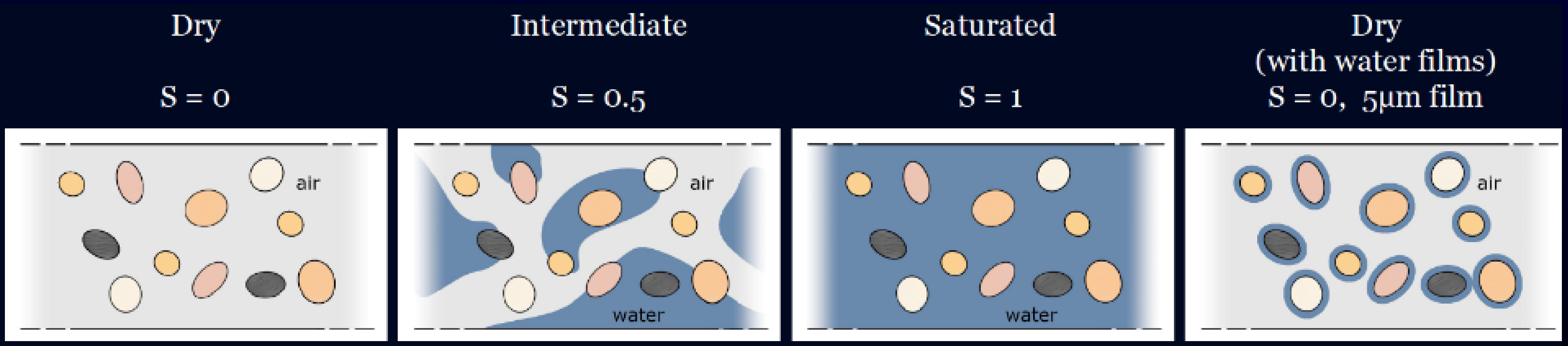
↓ ABM-B

↓ ABM-U


ABM-U
Incident Light
Scattered
Reflect/Refract
Adaxial
Epidermis
Reflect/Refract
Mesophyll
Absorption
Test
Absorption
Test
Reflect/Refract
Air
Absorbed
Reflect/Refract
Mesophyll
Absorption
Test
Absorption
Test
Reflect/Refract
Abaxial
Epidermis
Reflect/Refract
Scattered
Incident Light

- A model design can also evolve to enhance the fidelity/cost ratio of its predictions through:
  - the filtering of implementation “bugs”
  - the optimization of its algorithms
  - the incorporation of new features

Water Saturation States Considered by SPLITS-2



Schedule

- ✓ Introduction
- ✓ Biophysical Background
- ✓ Drawing Board
- ✓ Data Availability and Quality

Break

- ✓ Design Issues
- ❑ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

“Remember that all models are wrong; the practical question is how wrong do they have to be not to be useful.”

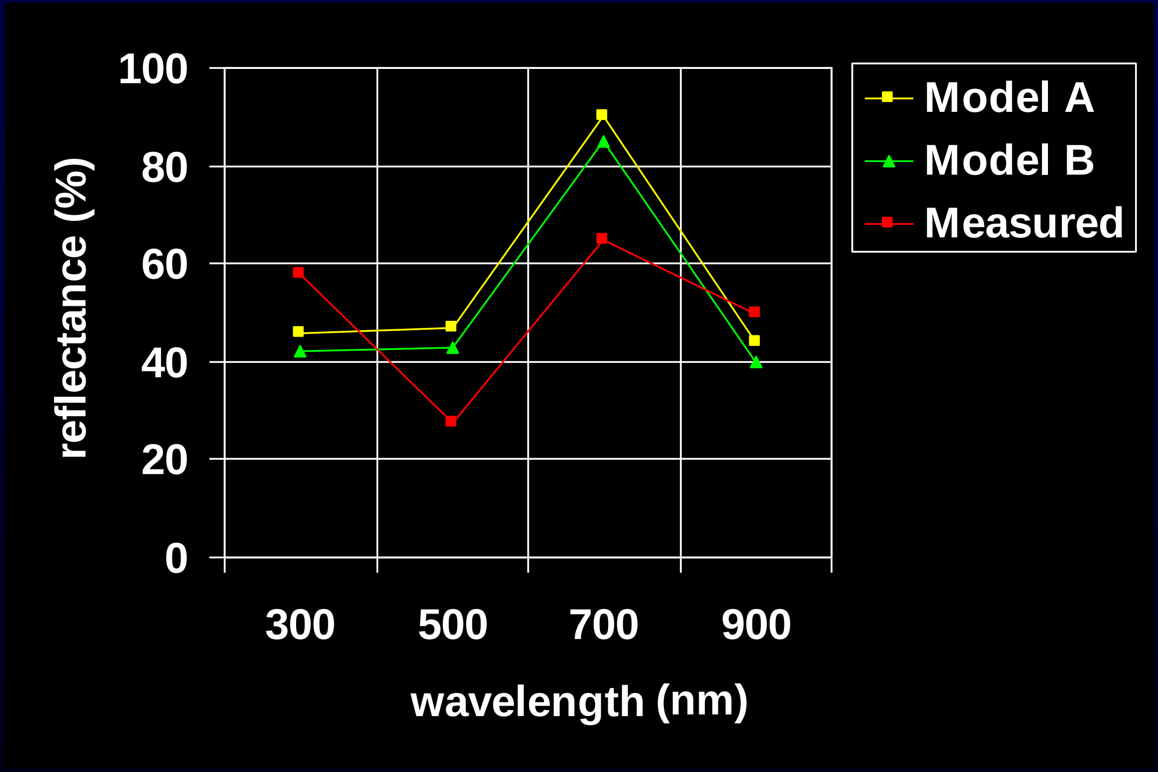
G. Box (1987)

Evaluation Approaches

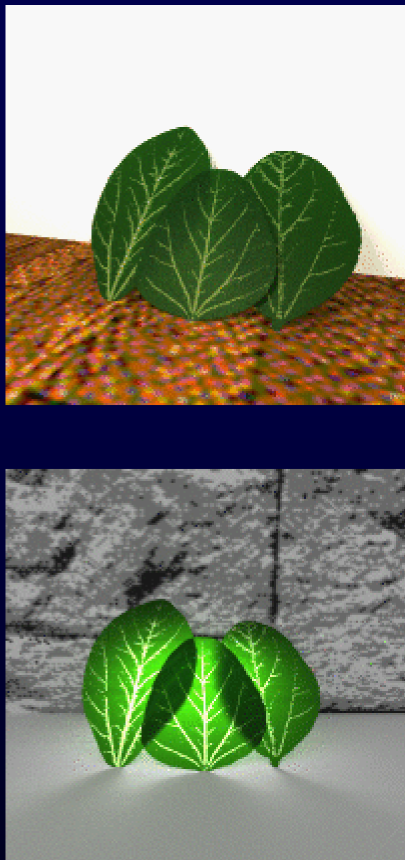
- Relative Comparisons
- Quantitative Comparisons
- Qualitative Comparisons
- Correctness vs. Efficiency

Relative Comparisons

- Comparisons with other models based on similar approaches



➢ Visual inspection

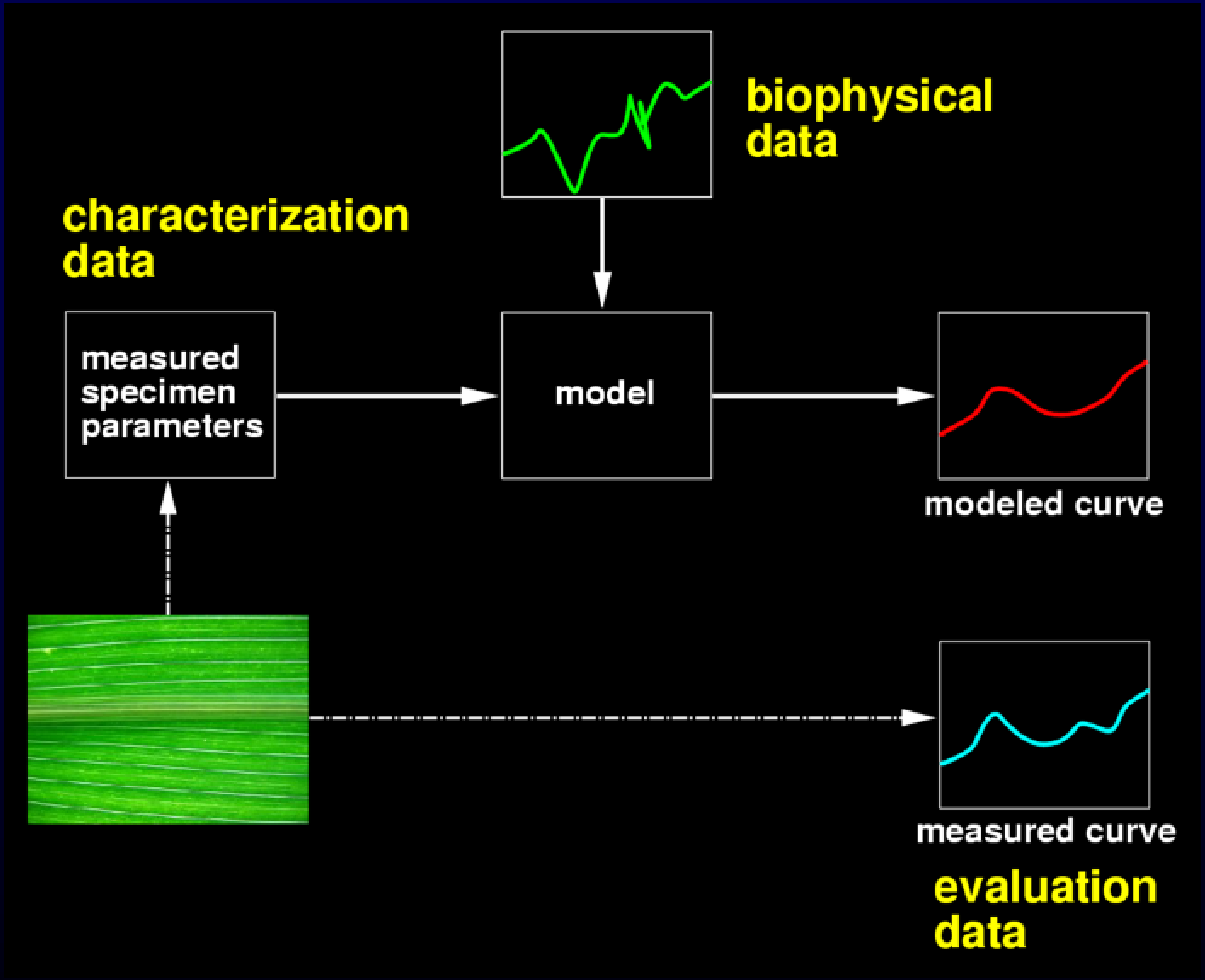


ABM

“Artistic” Colors

ABM-B

Quantitative Comparisons



- Reproduction of measurement (experimental) conditions as faithfully as possible

  - Specimens' (or samples') characterization data

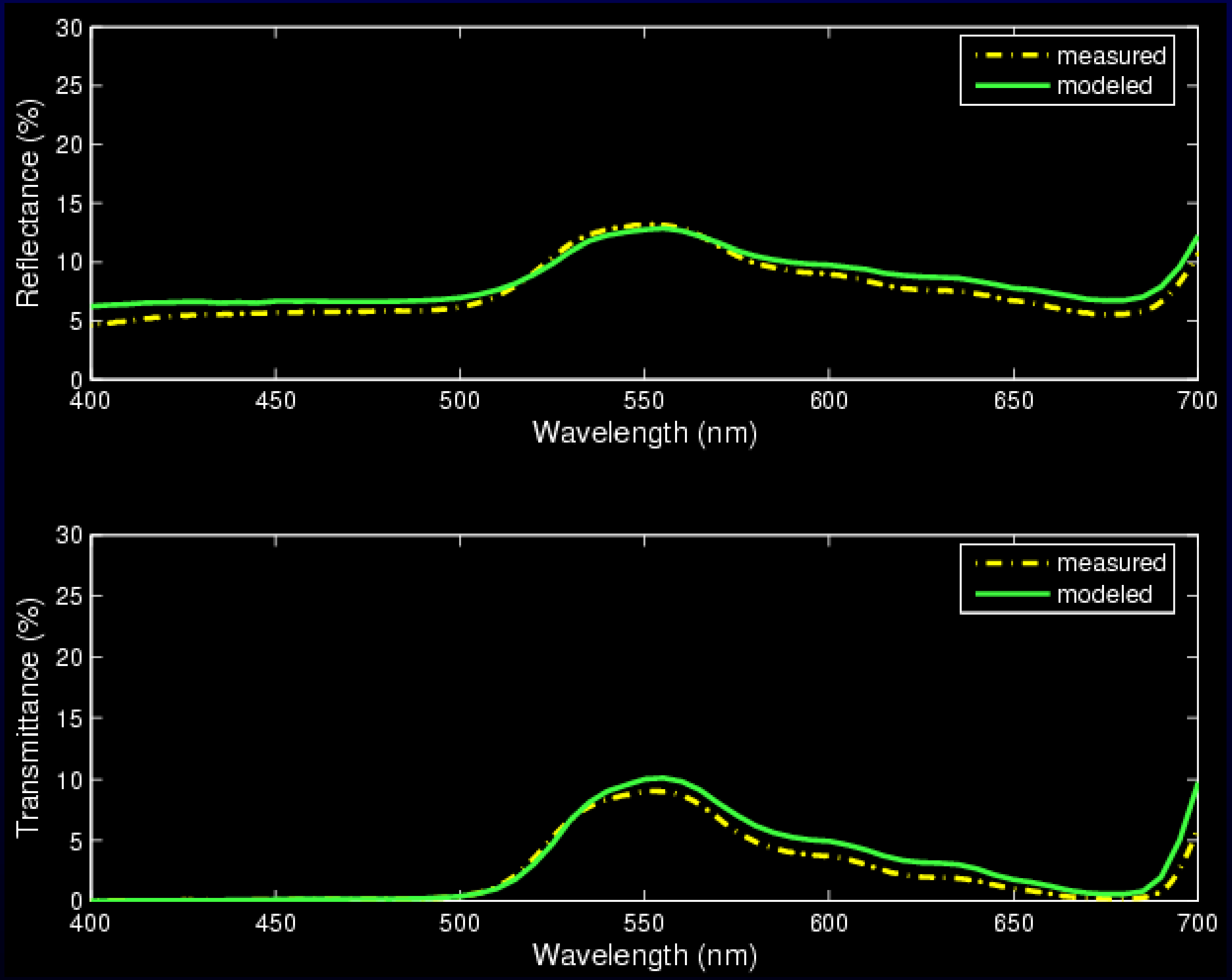
  - Incidence and viewing geometries

  - Actual devices' accuracy and precision

  - Proper implementation of virtual measurement devices

• “Direct” comparisons with measured data

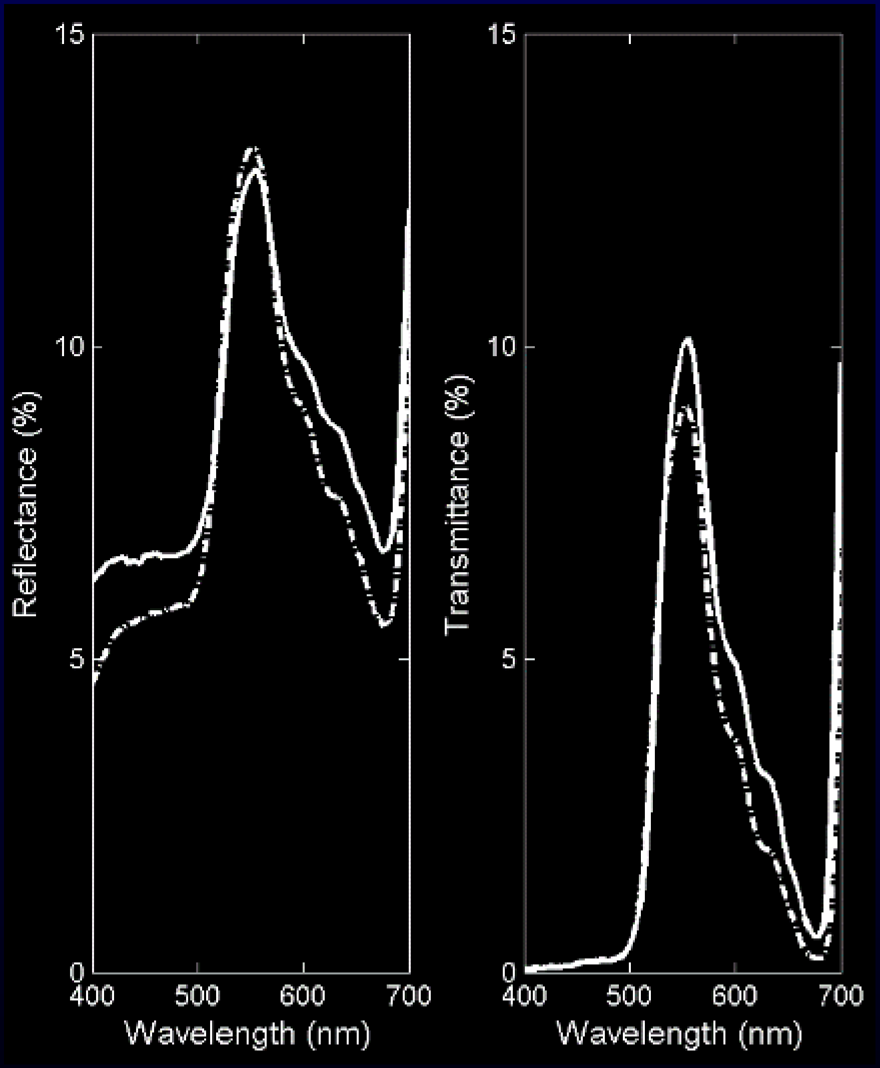
Modeled (ABM-U) and Measured (LOPEX) Spectral Signatures



LOPEX

ABM-U

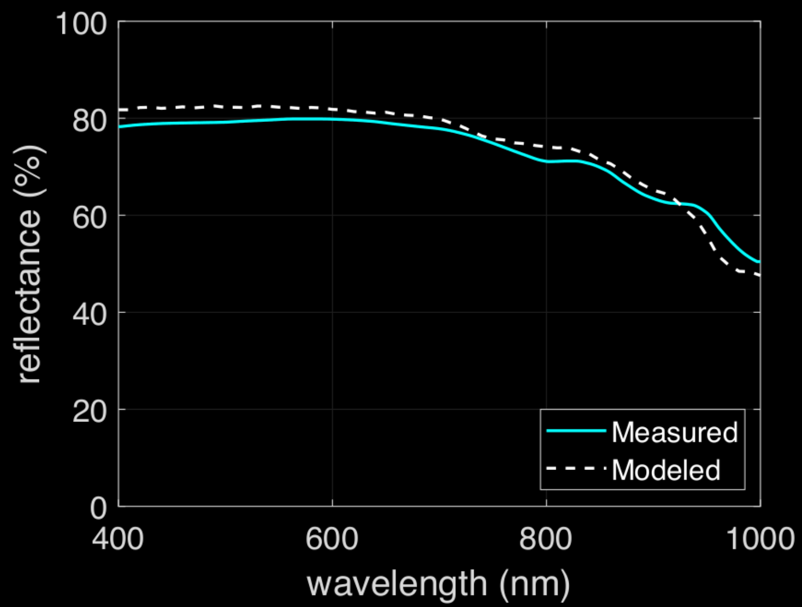
- Are the curves really close?



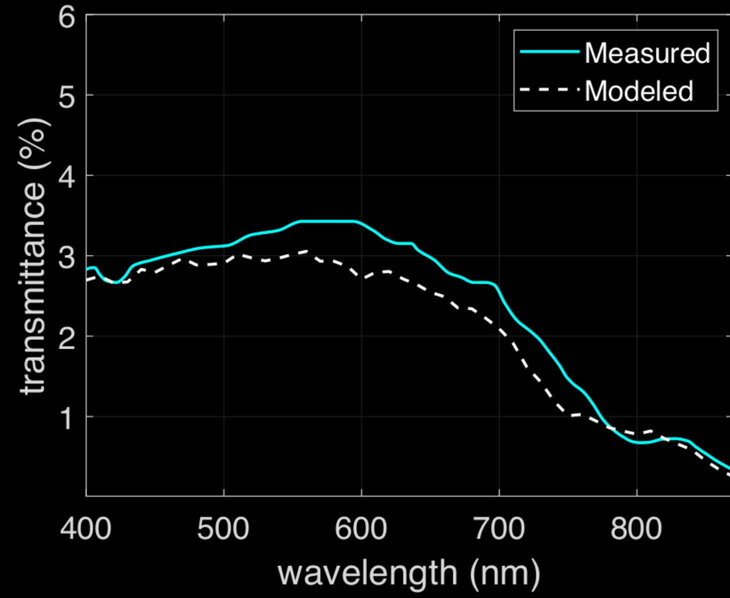
- Can we use an error metrics? Which one?

  - ❖ How about root mean square error (RMSE)?
  - ❖ Reflectance curve < 0.0096
  - ❖ Transmittance curve < 0.0093
  - ❖ Are these values “good” or “bad”? < 0.03

Modeled (SPLITSnow) and Measured (SISpec) Spectral Signatures



RMSE=0.0146



RMSE=0.0033

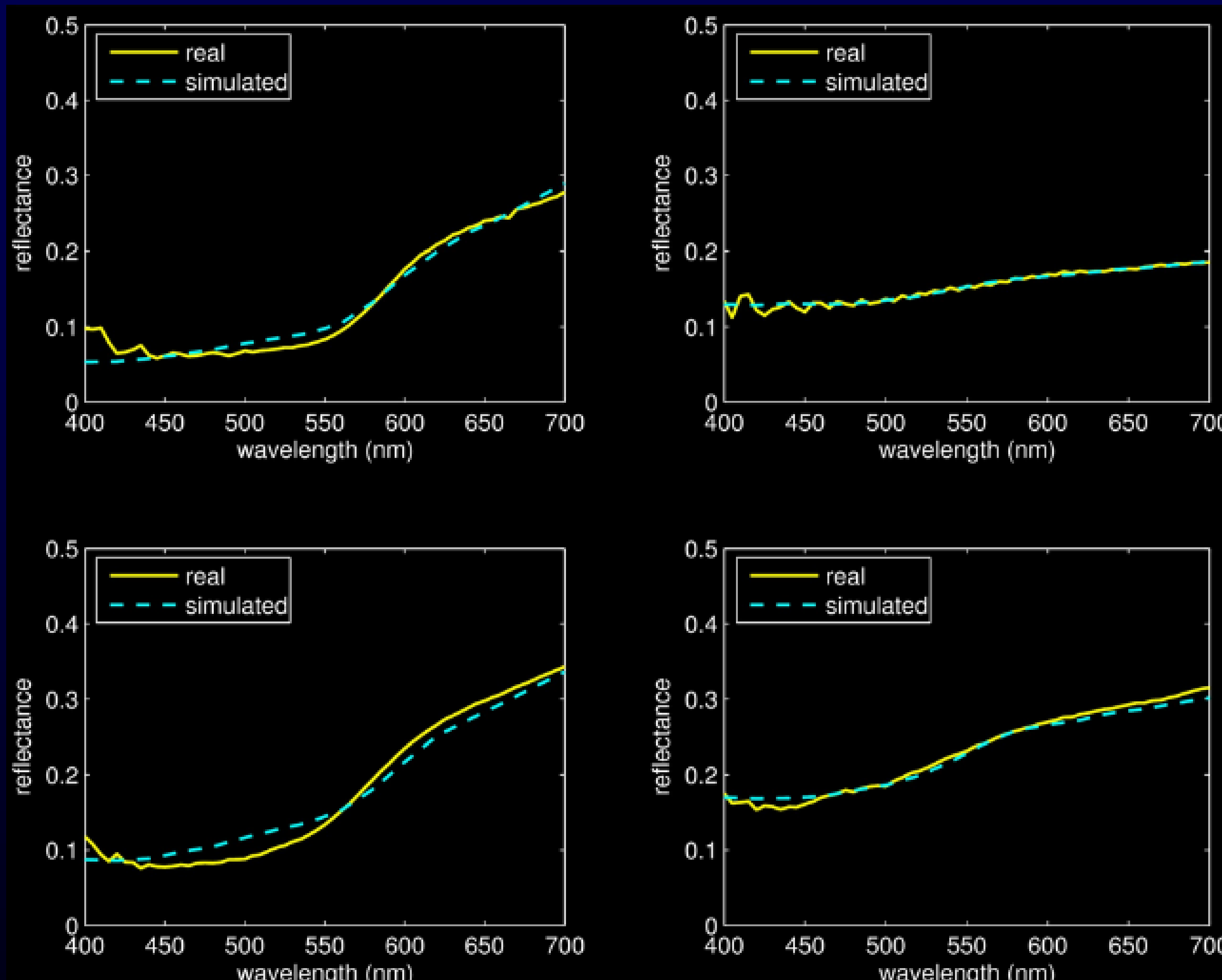
- What if exact values for key material parameters are missing?

  - We can search the parameter space for the best matches
  - Important: to keep the parameter values within valid ranges
  - We should specify the procedure used to select the values and how they are incorporated into the simulations
    - Fixed (*e.g.*, average values for refractive indices)
    - Variable (*e.g*., concentration of iron oxides in sand samples)

- Example: simulated (SPLITS) spectral signatures of sand samples

Dune sand
Australia
RMSE=0.0138

Beach sand
Peru
RMSE=0.0047



Dune sand
Saudi Arabia
RMSE=0.0166

Outcrop sand
USA
RMSE=0.0138

Qualitative Comparisons

- Based on visual observations of actual phenomena

ABM

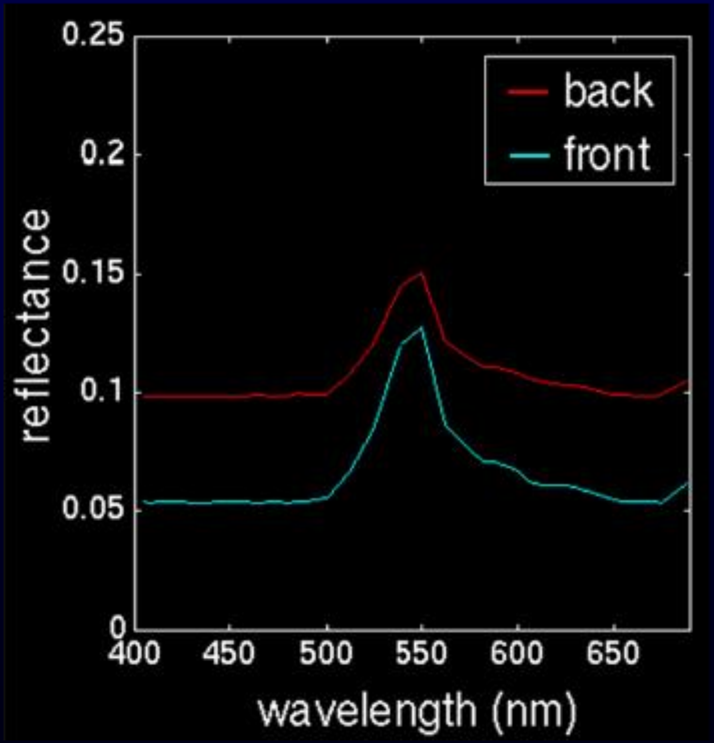
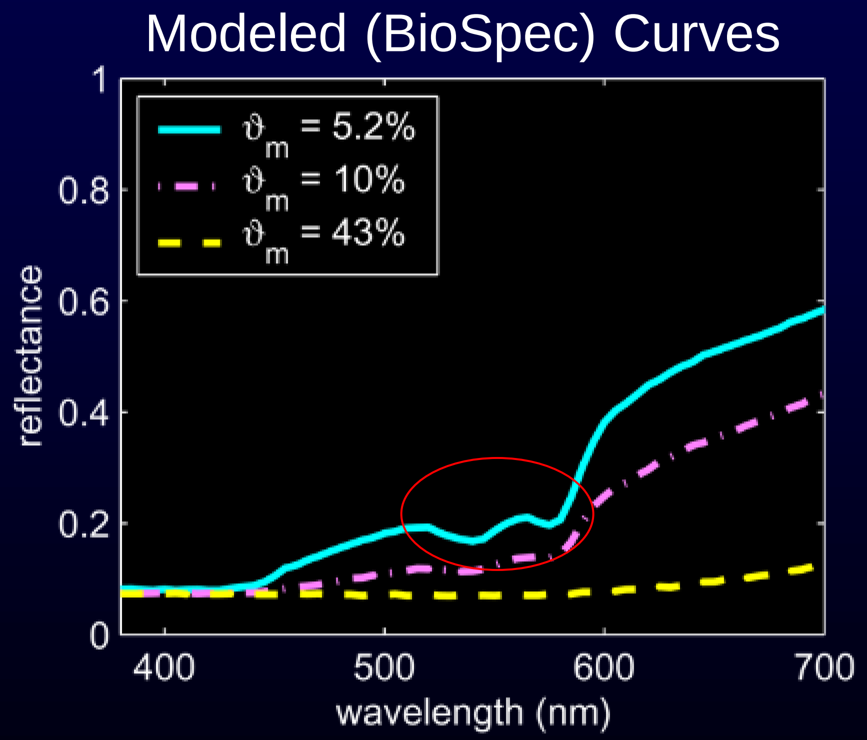


Photo of Soybean Leaves

- Based on experimental observations of actual phenomena
  - Characteristic spectral signatures
    - Example: effects of pigmentation on skin reflectance



➢ How effective are they?

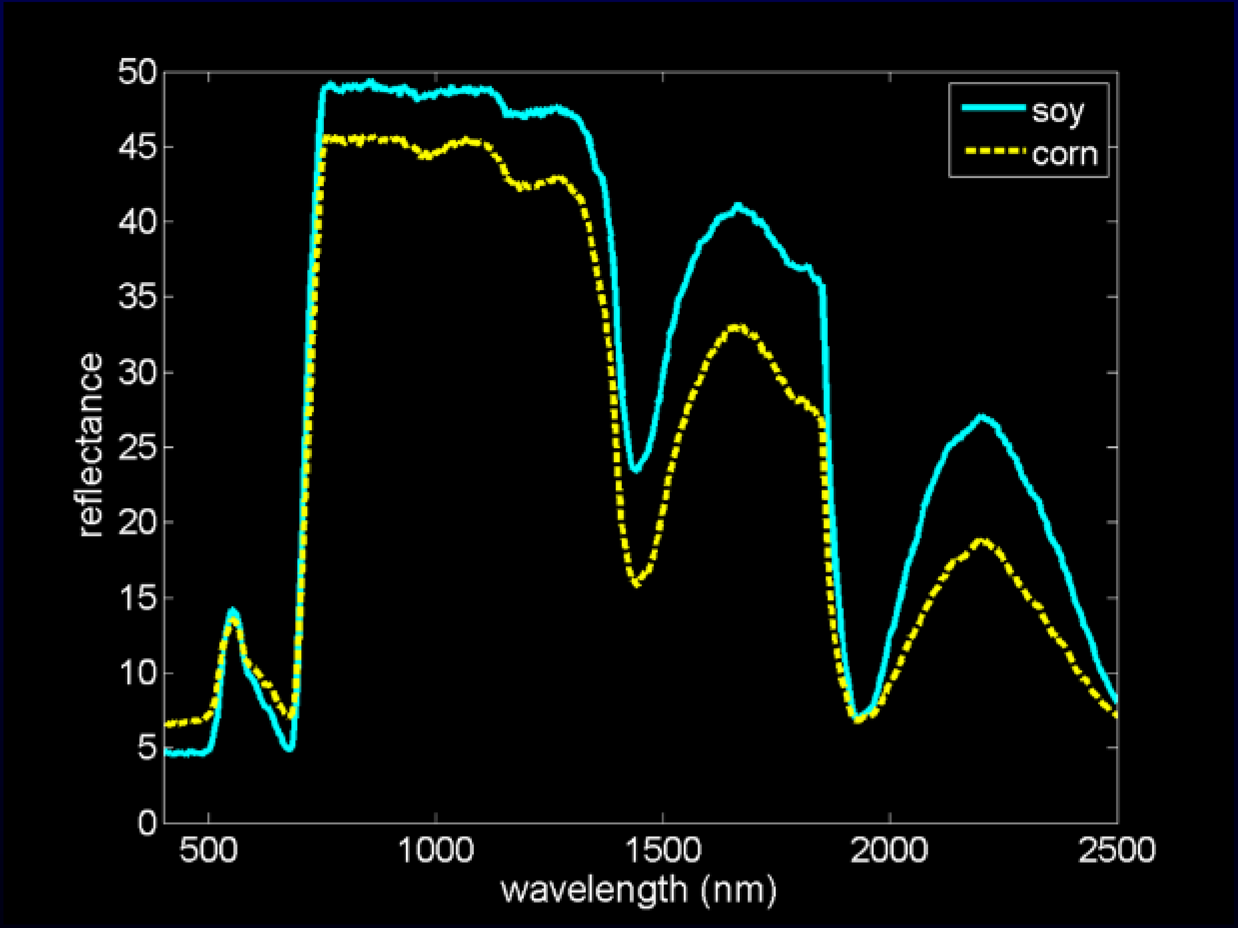
- They are less dependent on data availability issues
- They enable a broader assessment of the behaviour of a model under different conditions
- They are less susceptible to experimental fluctuations

Newsprint

Cork

- They may guide us in the right direction, but they are not sufficient to demonstrate the correctness of a model

Typical Foliar Reflectance Curves

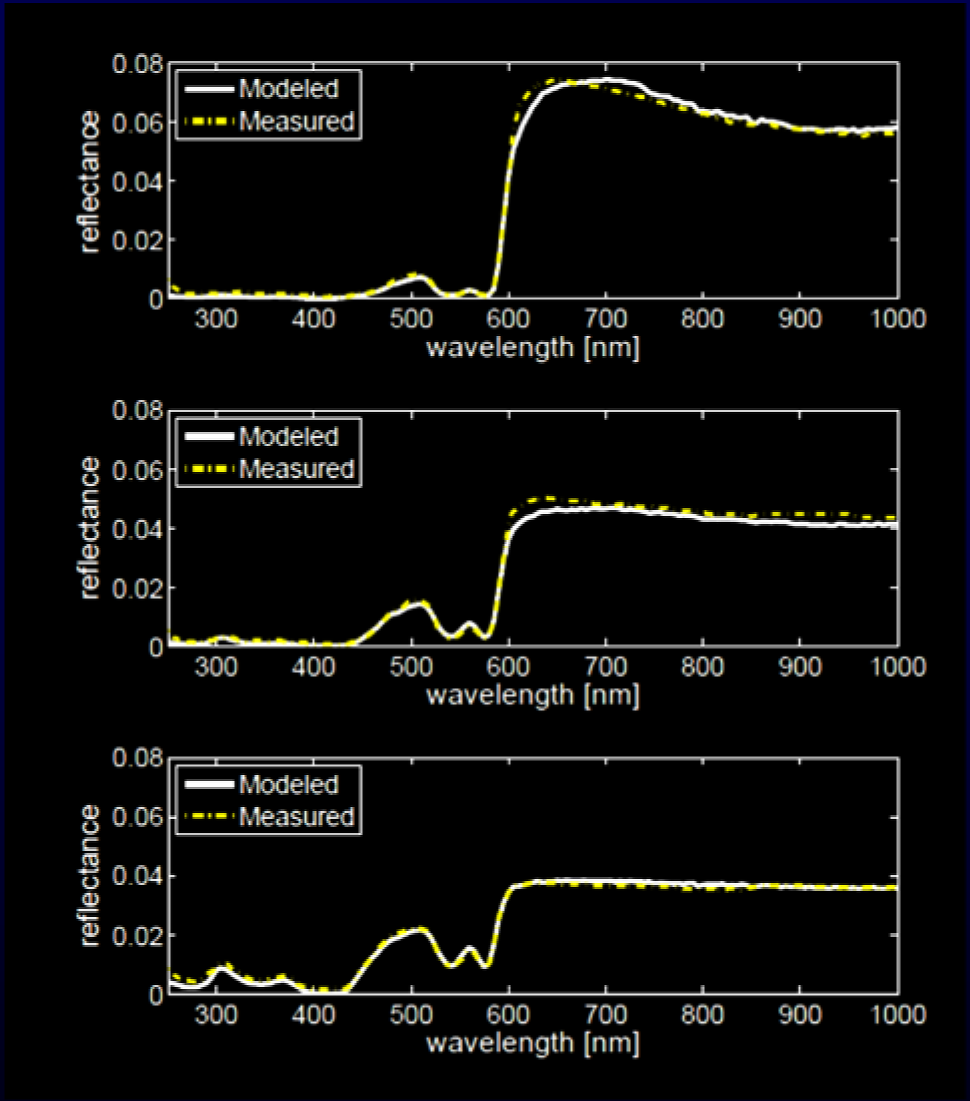


➢ General guidelines

- In conjunction, quantitative and qualitative comparison provide a more comprehensive picture of a model’s predictive capabilities

- In some instances, relevant quantitative and qualitative observations can come from the same set of experiments

Example: Blood Samples with Varying Hematocrit (HCT)



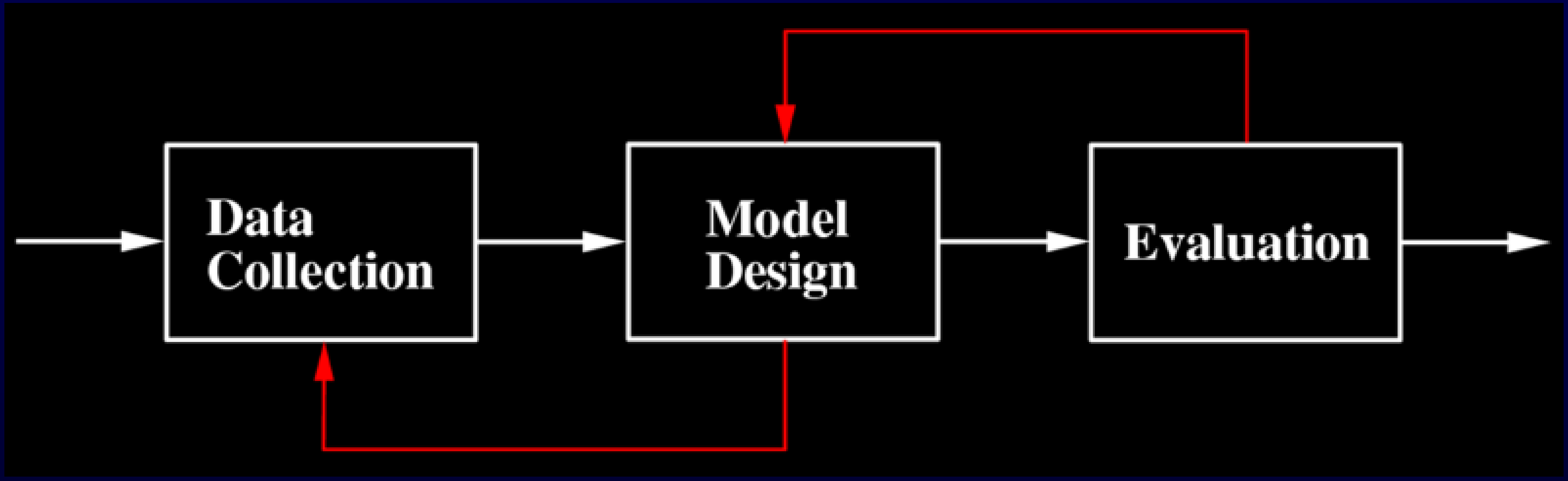
HCT = 0.33

HCT = 0.17

HCT = 0.084

(Measured data provided by Meinke *et al.*, Applied Spectroscopy 2005)

- Again, let’s recall the iterative nature of the model development process



- In short, quantitative and qualitative comparisons with the “real thing”:
  - rely on data availability
  - complement each other
  - facilitate the investigation of implementation errors
  - enable the iterative refinement of the algorithms
  - provide evidence of the fidelity of the simulations, but they may not represent a full proof of their correctness

Hyperspectral Modeling of Skin Appearance

Tenn F. Chen, Gladimir V. G. Baranoski
Bradley W. Kimmel, and Erik Miranda

Natural Phenomena Simulation Group
University of Waterloo

“… the idea is to try to give **all** of the information to help others to judge your contribution, not just the information that leads to judgment in one particular direction or another.”

R.P. Feynman on the *Principle of Scientific Integrity* (1974)

- Is this principle closely followed in practice?

- How about mistakes identified after publication?

Correctnes vs. Efficiency

- Offline schemes
  - Pre-computation strategies
  - Reconstruction techniques
    - ❖ Regression Analysis
    - ❖ Principal Component Analysis (PCA)
    - ❖ Piecewise Principal Component Analysis (PPCA)
    - ❖ Combination of PCA and regression analysis techniques

(Varsa & Baranoski, IEEE CG & A 2024)

- Online schemes
  - Code optimization
  - Parallel processing (software and hardware alternatives)

Cluster

Graphics Processing Unit

- Is either of these approaches the “magic bullet”?
- What if none can lead to the performance that we need?
- Perhaps one can also work around the requirements of a given application to obtain a high-fidelity to cost ratio

(Kravchenko *et al.*, CAVW 2017)

High-Fidelity Iridal Light Transport Simulations at Interactive Rates

Boris Kravchenko, Gladimir V.G. Baranoski,
Tenn F. Chen, Erik Miranda and
Spencer Van Leeuwen

Natural Phenomena Simulation Group
University of Waterloo

Schedule

- ✓ Introduction
- ✓ Biophysical Background
- ✓ Drawing Board
- ✓ Data Availability and Quality

Break

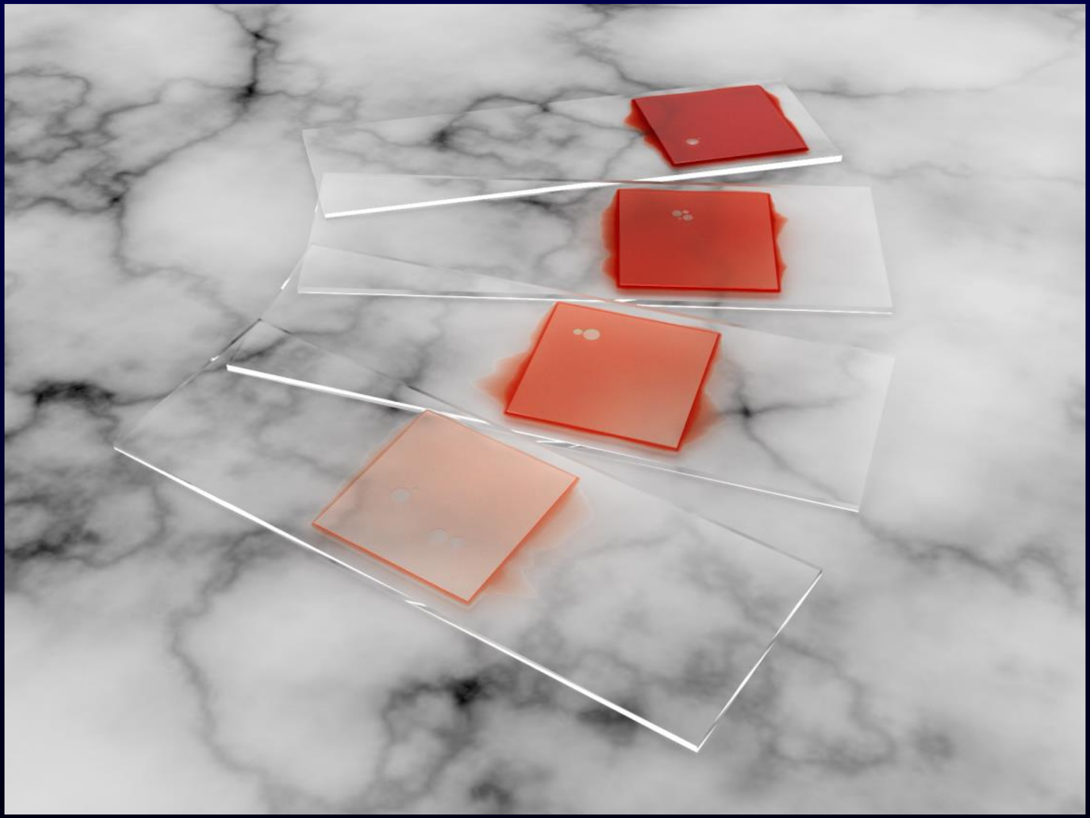
- ✓ Design Issues
- ✓ Evaluation Approaches
- ❑ Interdisciplinary Applications
- ❑ Conclusion

Interdisciplinary Applications

- Scope of Applications
- Case Studies
- Reproducibility

Scope of Applications

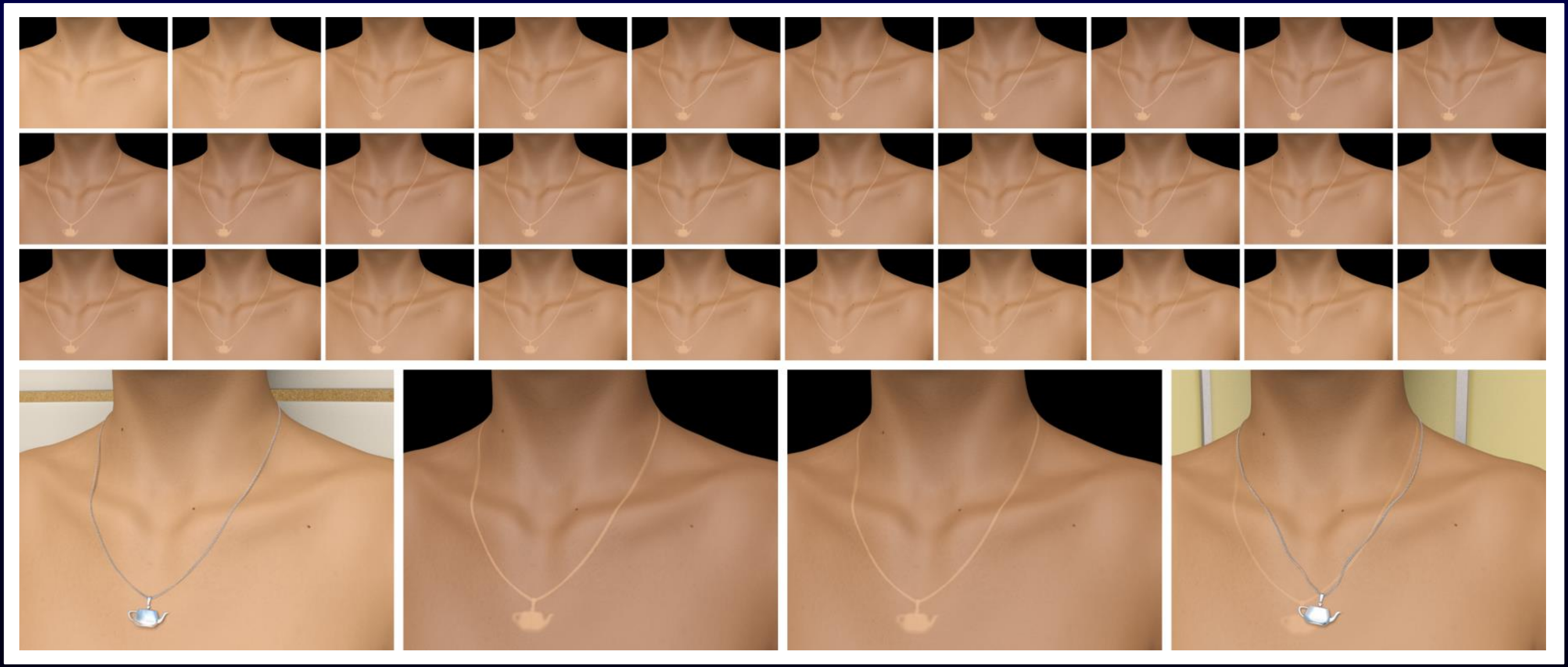
- From realistic image synthesis, …



➢ … photonics, …

- Investigation of photobiological processes triggered by light exposure

Tanning



(Chen & Baranoski, SPIE Photonics West 2019)

A Physiologically-Based Framework for the Simulation of Skin Tanning Dynamics

Tenn F. Chen and Gladimir V. G. Baranoski

Natural Phenomena Simulation Group

University of Waterloo

➢ … and biomedical optics ...

- Screening, treatment and monitoring of medical conditions

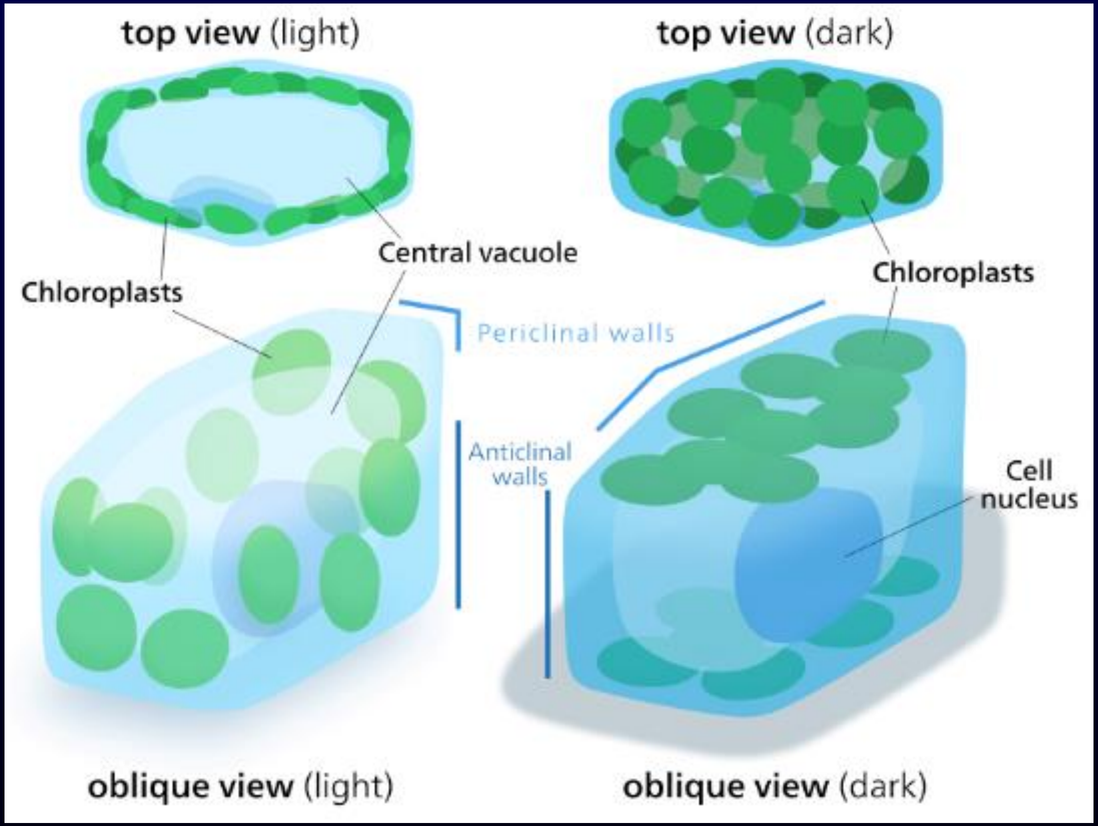
Jaundice

Phototherapy

  - "On the Effective Differentiation and Monitoring Variable Degrees of Hyperbilirubinemia Severity Through Noninvasive Screening Protocols" (Baranoski *et al*., IEEE Engineering in Medicine and Biology 2018)

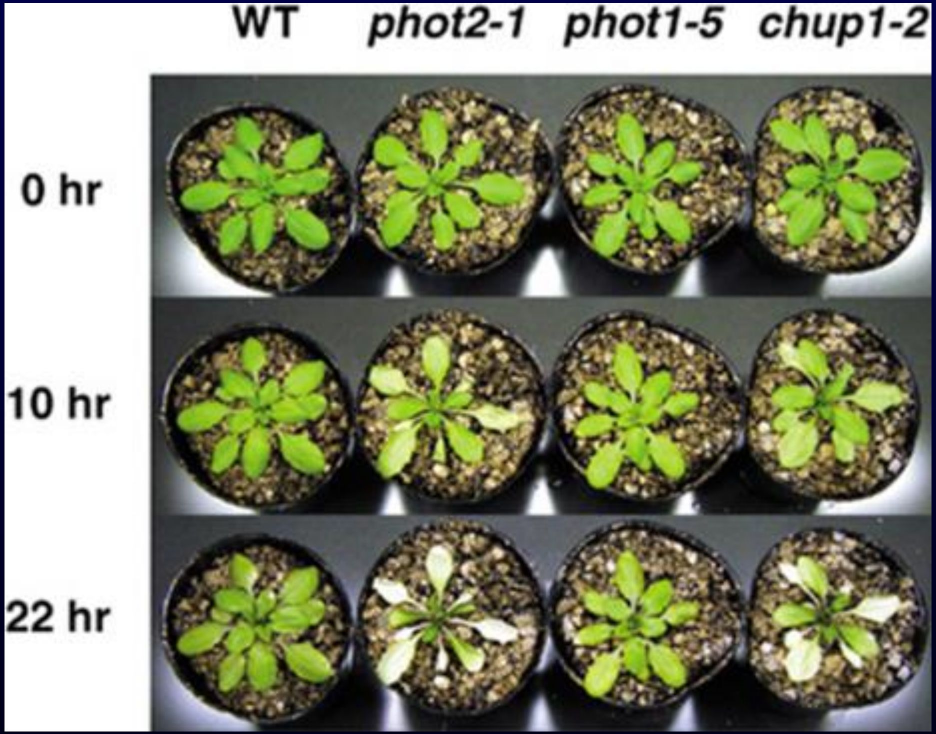
➢ … to systems biology, …

- Investigation of biophysical processes (*e.g.,* chloroplast movements) triggered by environmental stimuli



➢ … to systems biology, …

- Investigation of biophysical processes (*e.g.,* chloroplast movements) triggered by environmental stimuli



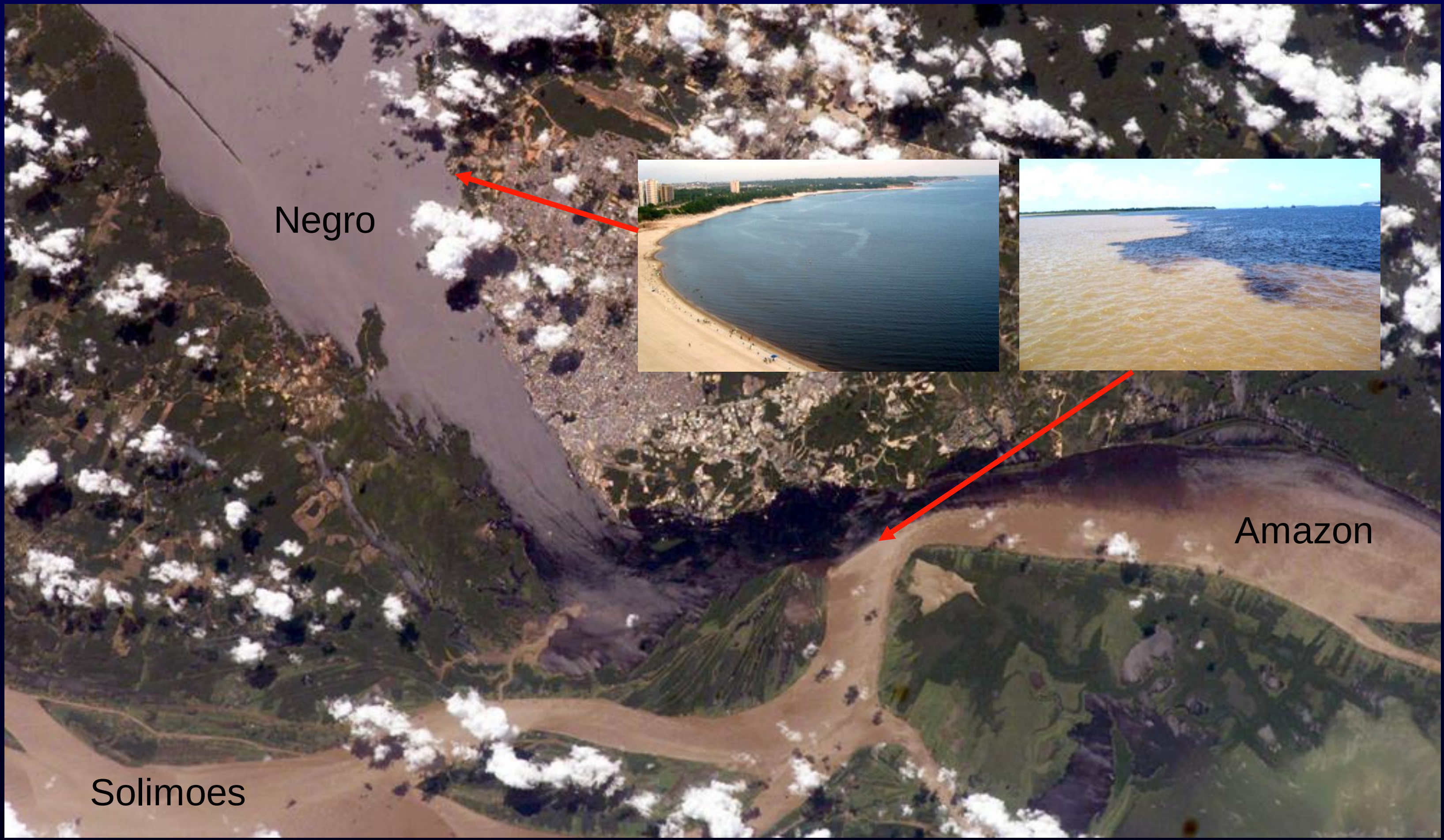
(Kasahara *et al.*, Nature 2002)

➢ … remote sensing, …

- Assessment of natural resources (*e.g*., fresh water)

Landsat Image of the Amazon Basin

Negro-Solimoes River Confluence at Manaus, Brazil



Photograph - ISS Crew Earth Observations Experiment

Negro river's dark color elicited by low silt content and humic acid produced by the incomplete breakdown of phenol-containing plants (organic matter)

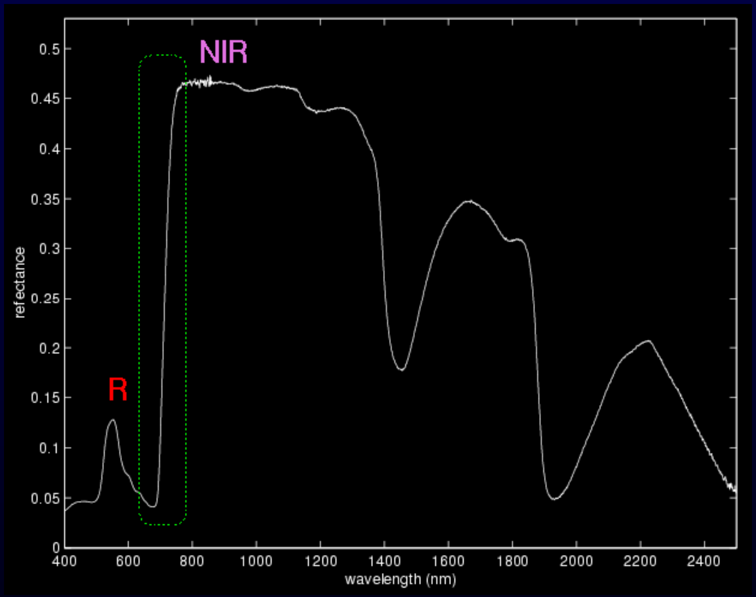
- Monitoring of natural hazards (*e.g*., avalanche risks)

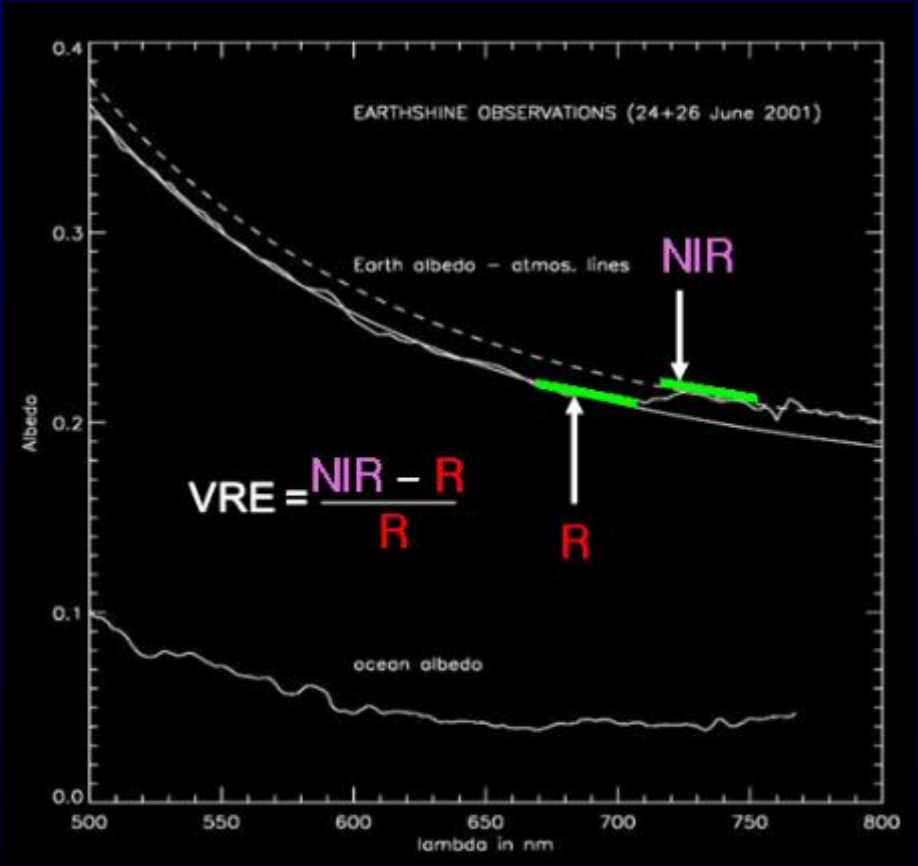
  - “*In silico* assessment of light penetration into snow: implications to the prediction of slab failures leading to avalanches” (Varsa & Baranoski, SPIE Remote Sensing 2021)

➢ … and exobiology

- Use of vegetation red edge (VRE) as a biosignature in the search for extraterrestrial life

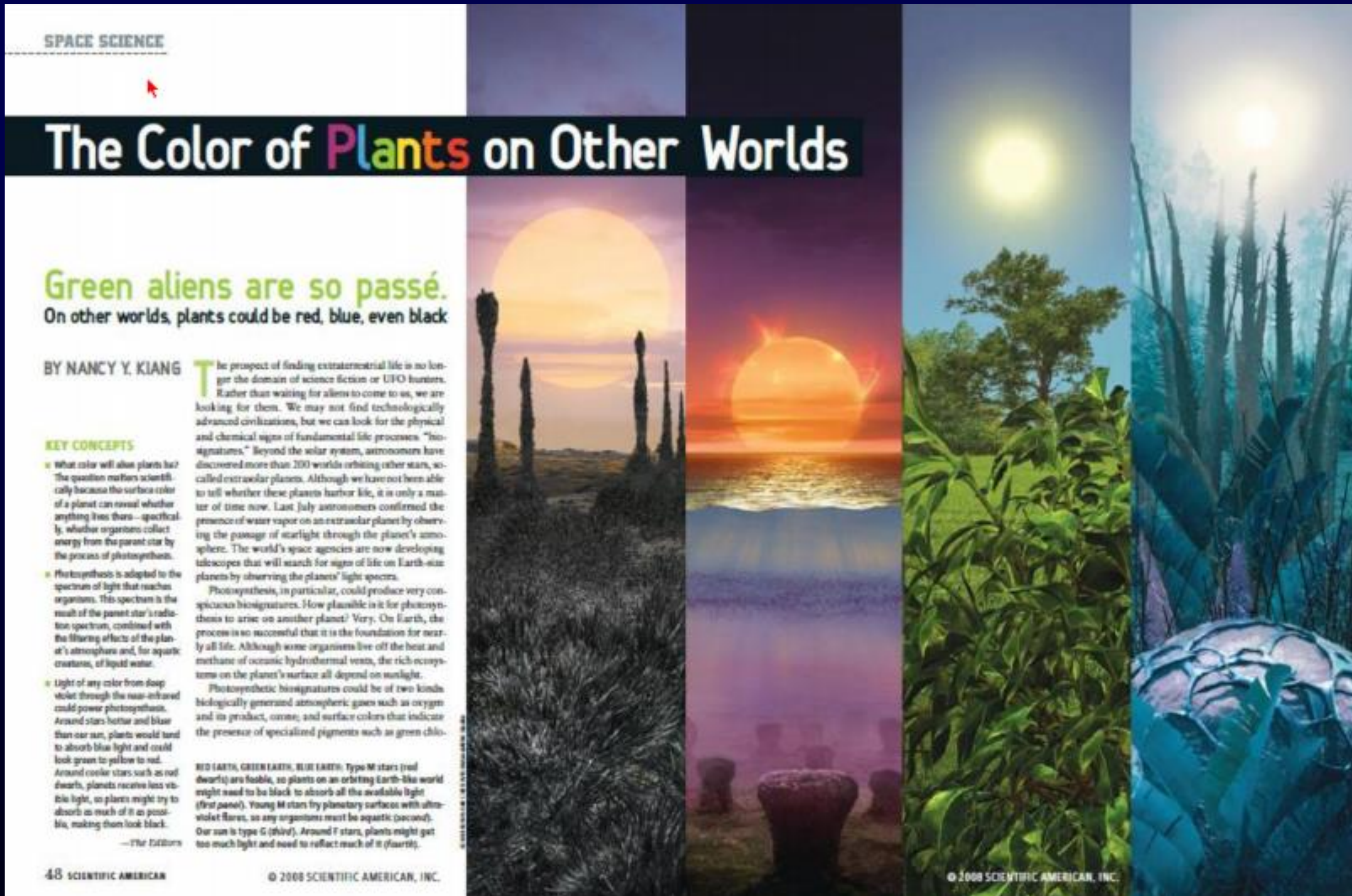
Leaf Reflectance





(Arnold *et al.*, Astronomy and Astrophysics 2002)

- Effects of extraterrestrial environments on living things



SPACE SCIENCE

The Color of Plants on Other Worlds

Green aliens are so passé.

On other worlds, plants could be red, blue, even black

BY NANCY Y. KIANG

The prospect of finding extraterrestrial life is no longer the domain of science fiction or UFO hunters. Rather than waiting for aliens to come to us, we are looking for them. We may not find technologically advanced civilizations, but we can look for the physical and chemical signs of fundamental life processes: "biosignatures." Beyond the solar system, astronomers have discovered more than 200 worlds orbiting other stars, so-called extrasolar planets. Although we have not been able to tell whether these planets harbor life, it is only a matter of time now. Last July astronomers confirmed the presence of water vapor on an extrasolar planet by observing the passage of starlight through the planet's atmosphere. The world's space agencies are now developing telescopes that will search for signs of life on Earth-size planets by observing the planets' light spectra.

Photosynthesis, in particular, could produce very conspicuous biosignatures. How plausible is it for photosynthesis to arise on another planet? Very. On Earth, the process is so successful that it is the foundation for nearly all life. Although some organisms live off the heat and methane of oceanic hydrothermal vents, the rich ecosystems on the planet's surface all depend on sunlight.

Photosynthetic biosignatures could be of two kinds: biologically generated atmospheric gases such as oxygen and its product, ozone; and surface colors that indicate the presence of specialized pigments such as green chlo-

KEY CONCEPTS

- What color will alien plants be? The question matters scientifically because the surface color of a planet can reveal whether anything lives there—specifically, whether organisms collect energy from the parent star by the process of photosynthesis.
- Photosynthesis is adapted to the spectrum of light that reaches organisms. This spectrum is the result of the parent star's radiation spectrum, combined with the filtering effects of the planet's atmosphere and, for aquatic creatures, of liquid water.
- Light of any color from deep violet through the near-infrared could power photosynthesis. Around stars hotter and bluer than our sun, plants would tend to absorb blue light and could look green to yellow to red. Around cooler stars such as red dwarfs, planets receive less visible light, so plants might try to absorb as much of it as possible, making them look black.

—The Editors

RED EARTH, GREEN EARTH, BLUE EARTH: Type M stars (red dwarfs) are feeble, so plants on an orbiting Earth-like world might need to be black to absorb all the available light (first panel). Young M stars fry planetary surfaces with ultraviolet flares, so any organisms must be aquatic (second). Our sun is type G (third). Around F stars, plants might get too much light and need to reflect much of it (fourth).

48 SCIENTIFIC AMERICAN

© 2008 SCIENTIFIC AMERICAN, INC.

© 2008 SCIENTIFIC AMERICAN, INC.

“The intrusion of computational biology into ‘wet’ laboratories is producing a quite revolution wherein simulation tools are used to complement experiments and accelerate the hypothesis generation and validation cycle of research.”

Di Ventura *et al.*

“From *in vivo* to *in silico* biology and back”, Nature 2006

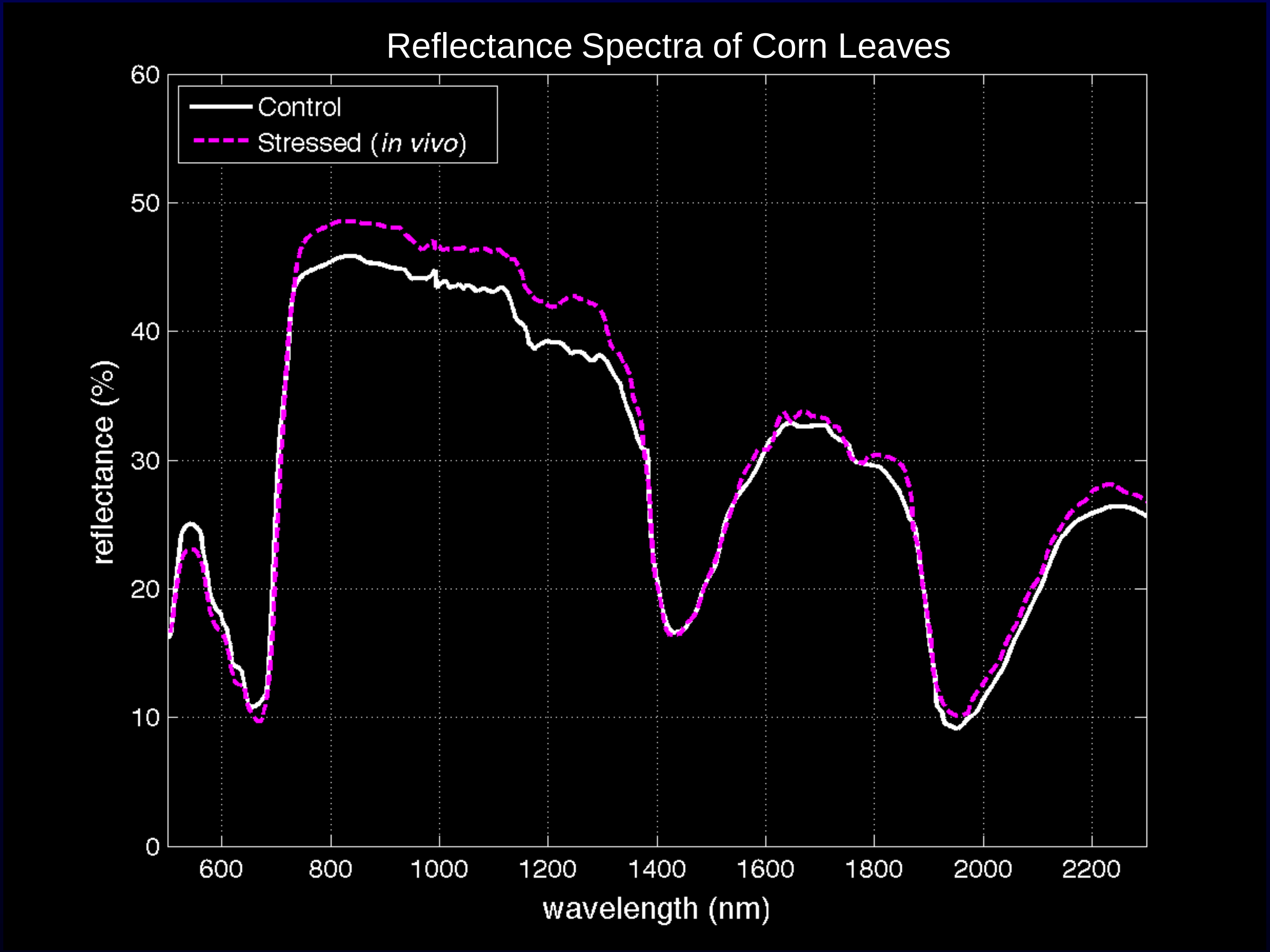
Case Study: Relocation of Chloroplasts

- Scientific context

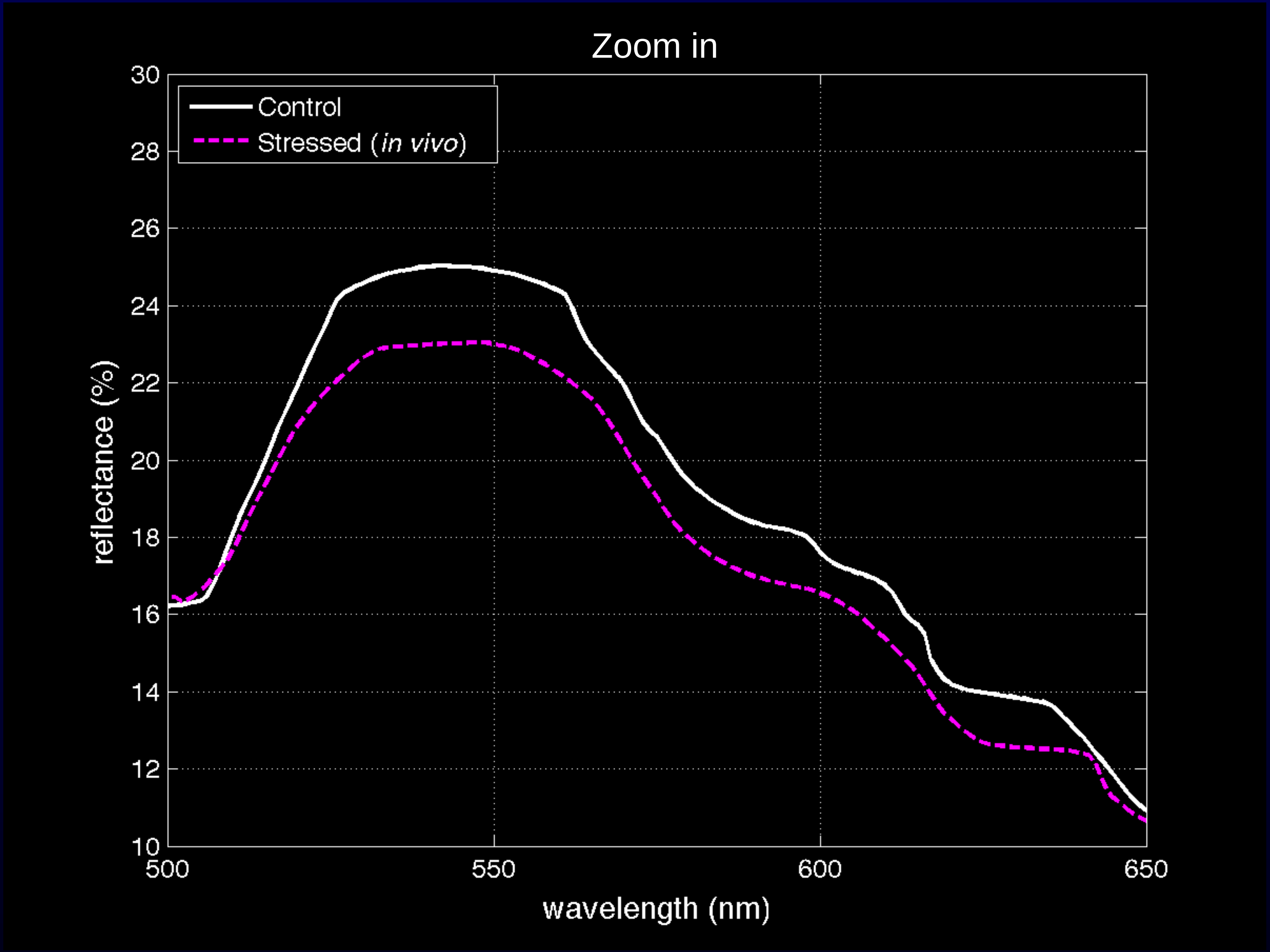
  - Apparently conflicting spectral responses measured for corn leaves under *in vitro* and *in vivo* water reduction procedures

  - Measurements performed by Thomas *et al.* (1971) show an increase in the reflectance (visible spectral domain) of corn leaves subjected to *in vitro* moderate (~25%) water reduction procedures

- Thomas *et al.* (1971) also observed that leaves of plant under moderate *in vivo* water stress may appear darker than fresh (control) leaves
  - Water stress may decrease reflectance under certain conditions
- Experiments by Maracci *et al.* (1991) show a reflectance decrease for corn leaves under moderate (*in vivo*) water stress (pigment content remained constant)
  - Need of further experiments to study this tendency



"Interpretation of Reflectance Spectra by Plant Physiological Parameters"
by Maracci *et al*., IEEE IGARSS 1991



"Interpretation of Reflectance Spectra by Plant Physiological Parameters"
by Maracci *et al*., IEEE IGARSS 1991

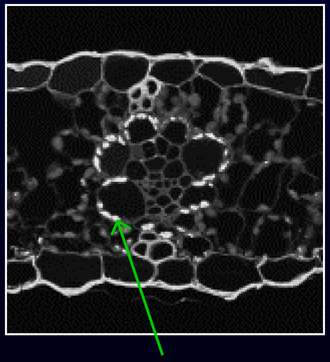
➢ Importance

- Increasing global demand of C_4 plants (*e.g.*, corn)
- Limited understanding about their adaptive mechanisms
- Need to develop more effective tools for the detection and monitoring of moderate water stress conditions

➢ Challenges

- Difficulties to conduct controlled experiments involving the same specimen under *in vitro* and *in vivo* moderate water reduction procedures

- *In situ* investigations of adaptive responses of C_4 plants, such as the relocation of chloroplasts due to an external stimulus, may affect the outcome of these responses with respect to other stimuli



- Possible explanation for the distinct responses of corn leaves

  - They may be elicited by intrinsic differences between *in vitro* and *in vivo* water reduction procedures

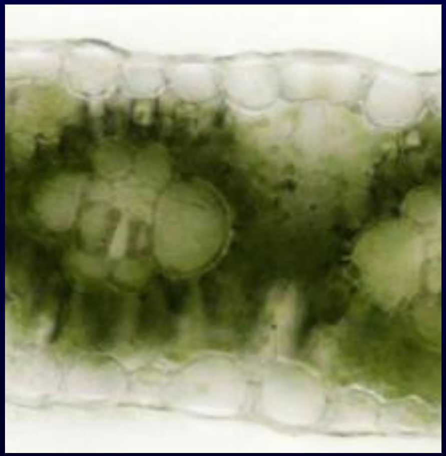
- *In silico* hypothesis formulation

  - Intensification of detour effects due to a more homogeneous distribution of chloroplasts triggered by water deficit signals

    - "*In silico* assessment of environmental factors affecting the spectral signature of C4 plants in the visible domain"
      (Baranoski *et al*., International Journal of Remote Sensing 2012)

- Recall that the detour effect increases absorption (in comparison with a homogeneous solution)

Leaf Cross-Section

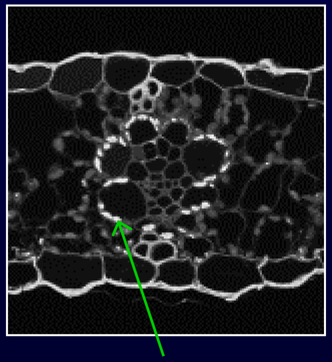


Chlorophyll Solution

➢ Simulation strategy

- Use the same characterization parameters for the *in vivo* and *in vitro* water reduced specimens

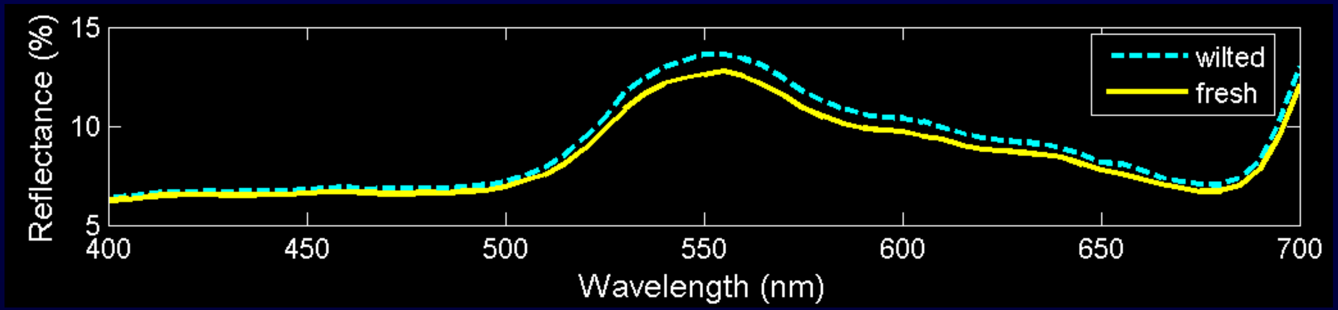
- ABM-U model incorporates a bound for angular light (ray) deviations caused by the heterogeneous distribution of chloroplasts



- Remove the bound for angular deviations in the case of *in vivo* water stressed specimens

➢ Qualitative agreement with measured data for ***in vitro*** water wilted (25%) leaves (Thomas *et al.* 1971)

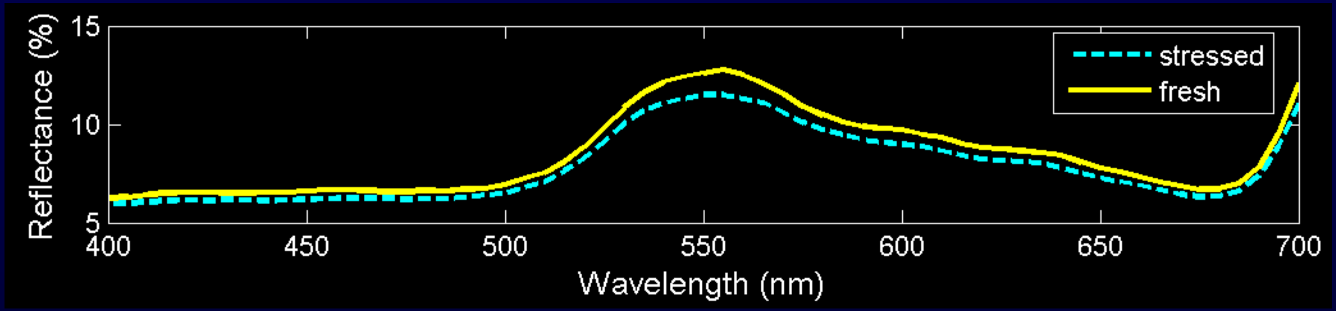
Modeled (ABM-U) Reflectance Curves



- Higher reflectance for the water wilted specimen
- More pronounced reflectance increase around 550nm

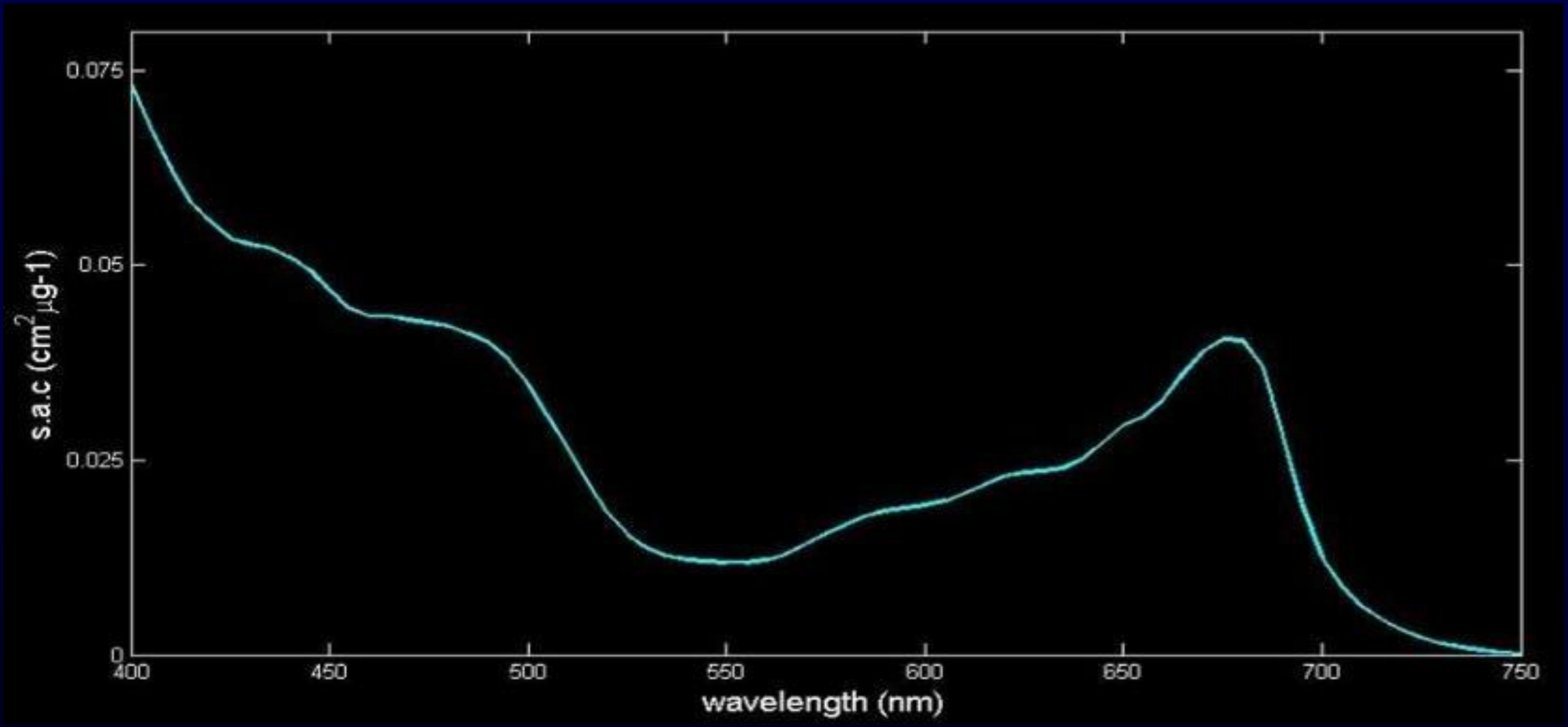
➢ Qualitative agreement with measured data for ***in vivo*** water stressed (25%) leaves (Maracci *et al.* 1991)

Modeled (ABM-U) Reflectance Curves



- Lower reflectance for the water stressed specimen
- More pronounced reflectance decrease around 550nm

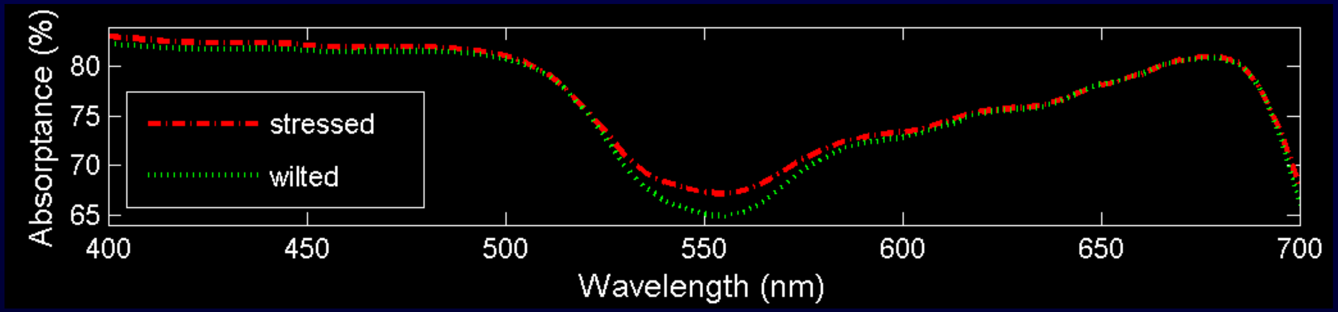
- Recall that the detour effect increases absorption, and the increase is more pronounced in bands of absorption minima (around 550nm for chlorophyll)



Absorption Spectra for chlorophyll a+b
(Jacquemoud *et al*., RSE 1996)

- Qualitative comparison of modeled bihemispherical absorptance values for wilted (***in vitro*** water reduction) and stressed (***in vivo*** water reduction) specimens

Modeled (ABM-U) Absorptance Curves



- Higher absorptance for the ***in vivo*** water stressed specimen in the photosynthetic region around 550nm

- Can water deficit signals trigger the rerrangement of chloroplasts in corn leaves?

- If so, can the same mechanism be found in other C_4 plants (*e.g.*, sugarcane)?

- More wet lab experiments are required to confirm or refute this hypothesis

Case Study: Veins' Bluish Appearance and Rayleigh Scattering

- Scientific context

  - "The pigments and color of living human skin" by Edwards & Duntley (1939): suggestion of Rayleigh scattering in the skin

  - "Origins of tissue optical properties in the UVA, visible, and NIR regions" by Jacques (1996): suggestion that fibrils in the dermis can cause Rayleigh scattering

  - "Why do veins appear blue? A new look at an old question" by Kienle *et al.* (1996): no reference to Rayleigh scattering

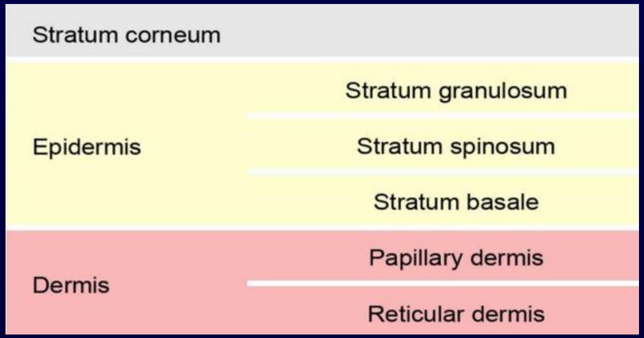
➢ Importance

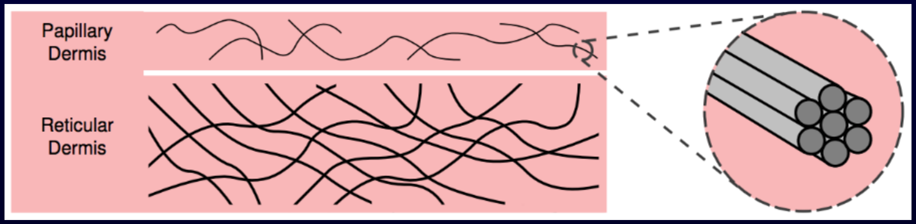
- Light attentuation phenomena eliciting the vein’s bluish apperance are also linked to skin’s fundamental optical processes

- A deeper understanding about these processes can lead to more effective methodologies and devices aimed at:
  - the noninvasive detection of physiological changes affecting the appearance of human skin
  - the early diagnosis and treatment of medical conditions associated with blood disorders

➢ Challenges

- Intrinsic limitations of *in situ* and *in vivo* experiments
  - Placement of sensors within thin skin layers (*e.g.*, papillary dermis)
  - Comprehensive characterization of skin specimens
  - Alteration of skin morphology (*e.g.*, dermal fibers and fibrils)





- To achieve an appropriate level of variability, many subjects would be required, which may not be practical

- Possible explanation for the bluish appearance of veins
  - Light scattering by papillary fibrils prevents blue light from reaching the subcutaneous veins
  - A high percentage of red light is absorbed within the veins

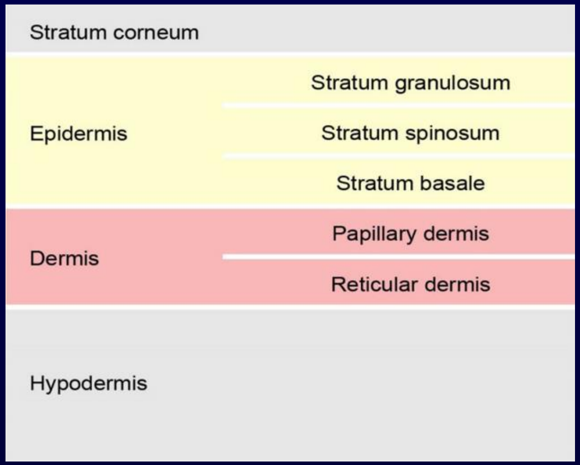
- *In silico* hypothesis formulation
  - Rayleigh scattering elicited by collagen fibrils within the papillary dermis plays a pivotal role in the veins' appearance
    - "Elucidating the contribution of Rayleigh scattering to the bluish appearance of veins" (Van Leeuwen & Baranoski, Journal of Biomedical Optics 2018)

➢ Simulation strategy

- Use HyLIoS and CLBlood models

- Consider two scenarios

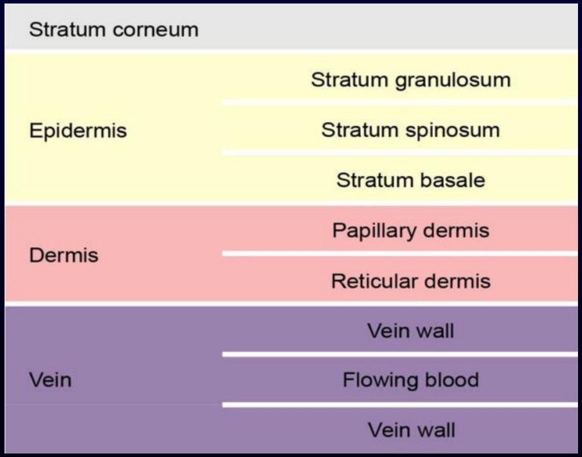
  - Without a subcutaneous vein: hypodermis representation reflects all light reaching it



  - With a subcutaneous vein:

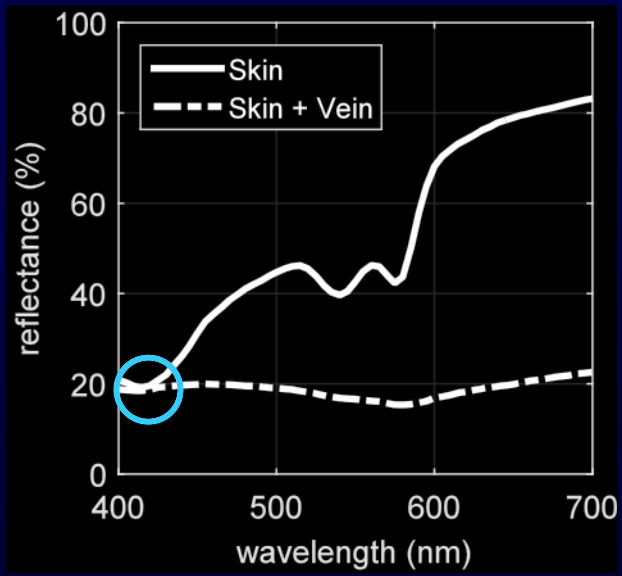
    - ❖ vein wall characterized by its refractive index

    - ❖ flowing blood & light interactions handled by the CLBlood model

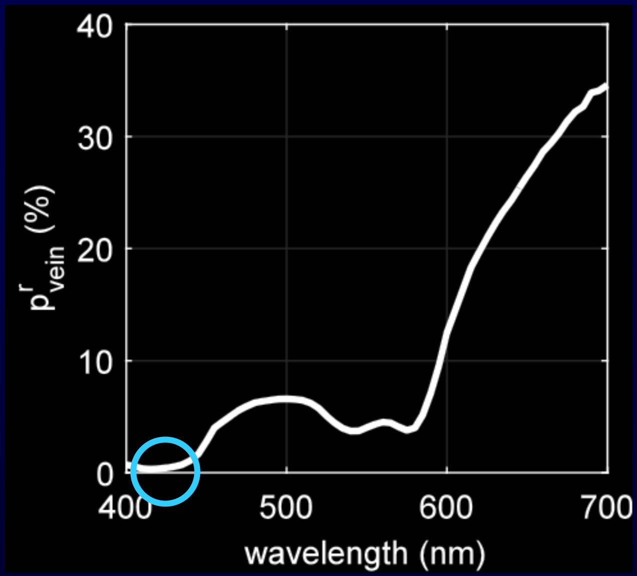


➢ Baseline experiments

Skin with and without Vein



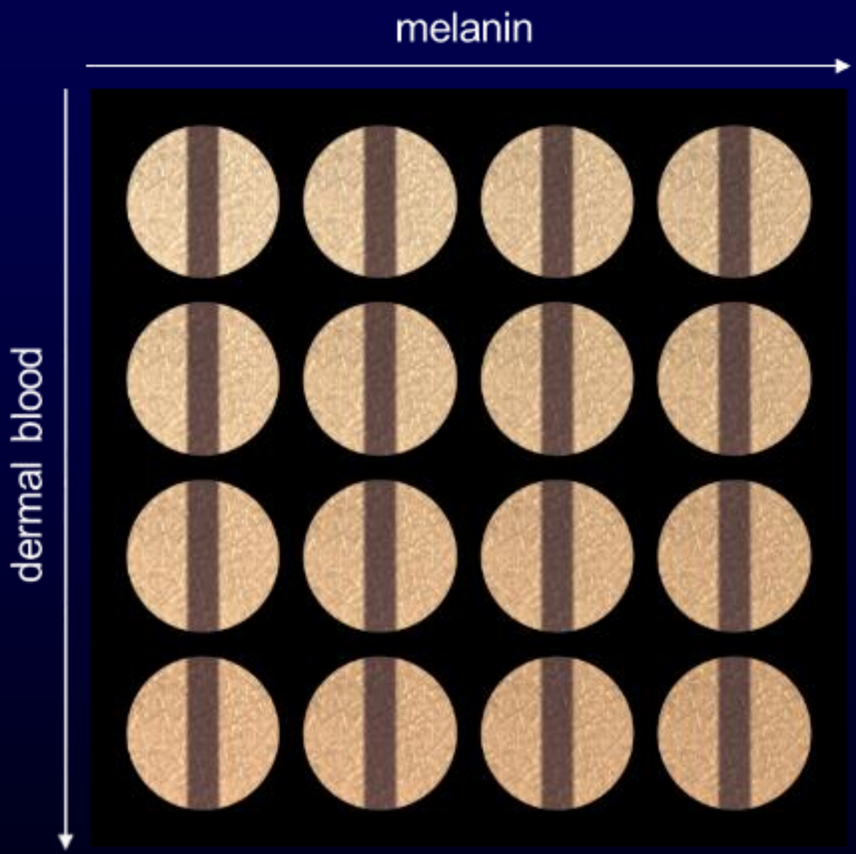
Isolated Vein



- Blue light is scattered before reaching the vein
- The vein would absorb all light in the blue region

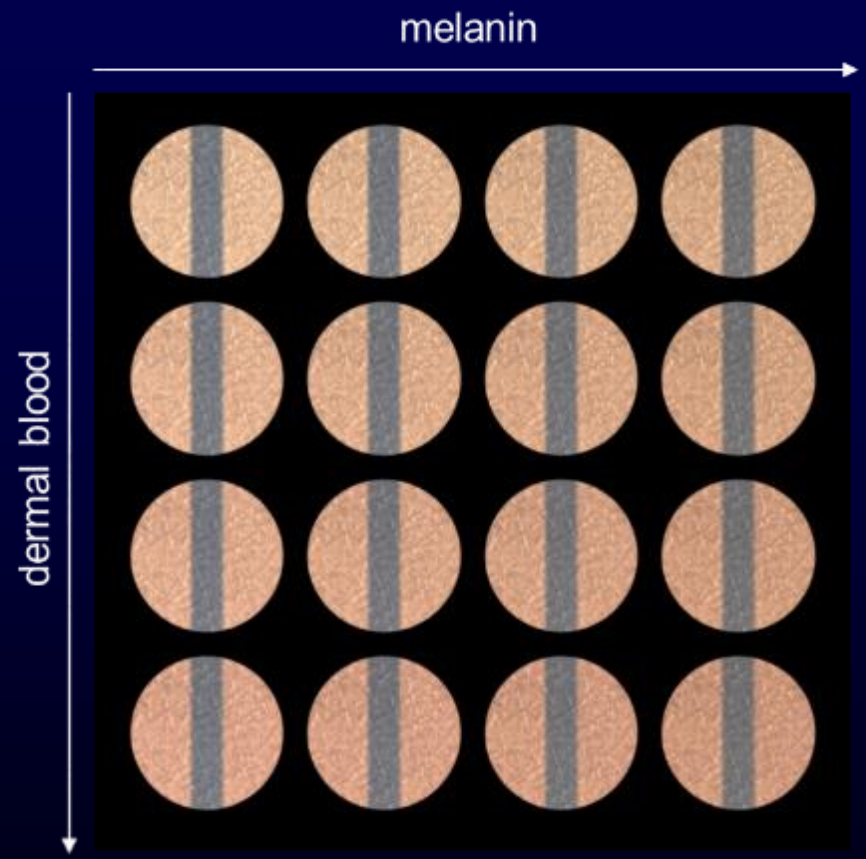
➢ Appearance experiments with varying pigment contents

Rayleigh scattering deactivated



swatches generated using
illuminant D65

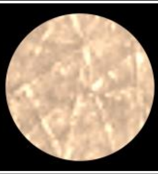
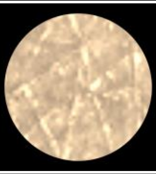
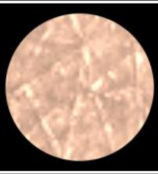
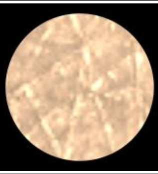
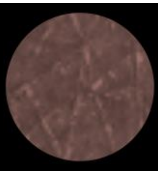
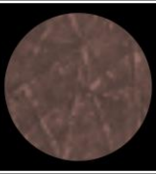
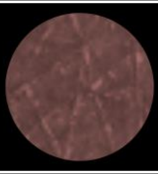
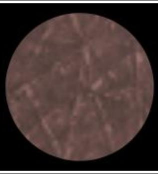
Rayleigh scattering activated



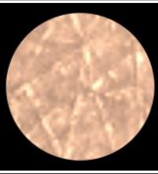
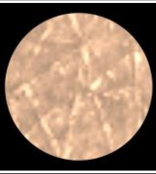
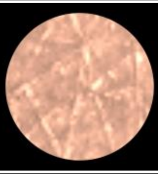
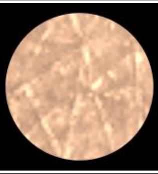
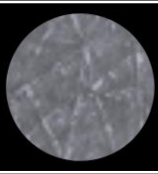
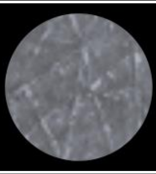
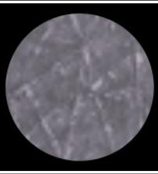
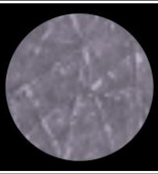
swatches generated using
illuminant D65

➢ Appearance experiments with distinct illuminants

Rayleigh scattering deactivated

Without a subcutaneous vein				
With a subcutaneous vein				
Illuminant	D50	D65	A	F2

Rayleigh scattering activated

Without a subcutaneous vein				
With a subcutaneous vein				
Illuminant	D50	D65	A	F2

- What these findings have indicated?
  - How the blue light is being scattered:
    Rayleigh scattering
  - What is scattering the blue light:
    Fibrils composing structural fibers
  - Where the blue light is being scattered:
    Papillary dermis
- The hypothesis is viable, but it is still subject to *in situ* validation when the required technology becomes available

Case Study: Density Effects on Snow Transmittance

➢ Scientific context

- Apparently conflicting reports about the impact of density on light transmission through snow

- Several research papers state that the transmittance of a snowpack increases following an increase in its density
  - Gerdel (1941), Curl *et al.* (1972), Richardson & Salisburry (1977), Saarinen *et al.* (2016), Robson and Aphalo (2019) …

- Experiments involving other granular materials suggest the opposite: transmittance decreases with increased density

➢ Importance

- Estimations of snow water equivalent (SWE)
- Impact on the spectral quality of light reaching subnivean vegetation and increasing its productivity (greening)
- Feedback effects negatively reinforcing climate changes

➢ Challenges

- Intrinsic limitations of *in situ* experiments
  - While attempting to place a sensor within a snow layer, one may inadvertently disturb the structure of the snowpack
  - Controlled parameter variations are difficult to be achieved when material changes are elicited by environmental factors that may affect multiple nivological characteristics simultaneously

- While controlled parameter variations can be attempted under laboratory conditions, artificially prepared samples lack the morphological diversity found in natural samples

- Possible explanation for the density “contradiction”

  - Aspects overlooked in the original field observations by Gerdel (1941) about the transmittance-density relationship

- *In silico* hypothesis formulation

  - The individual role played by density on snow transmittance variations can be masked by other nivological characteristics

    - “Environmentally-Induced Snow Transmittance Variations in the Photosynthetic Spectral Domain: Photobiological Implications for Subnivean Vegetation under Climate Warming Conditions” (Baranoski & Varsa, Remote Sensing 2024)

➢ Simulation strategy

- Conduct controlled *in silico* experiments using the SPLITSnow model and virtual snow samples with a characterization based on real snowpacks

- Follow specific guidelines for selecting snowpack data
  - Provenance: snowpacks from regions more sensitive to climate warming effects and less susceptible to contamination (*e.g*., Artic)
  - Availability of measured radiometric datasets (to be used as baseline references) accompanied by the snowpacks' detailed descriptions

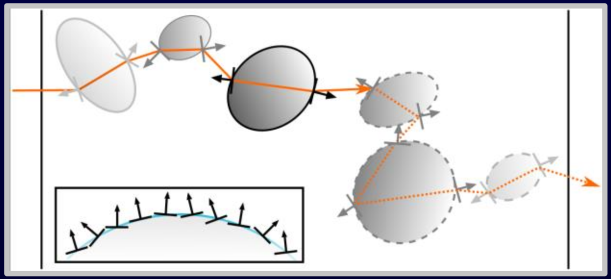
- Select snowpacks: located in the Svalbard island (Artic) and with radiometric data available in the SISpec database

➢ Simulation strategy

In Silico Experiments

Data Survey

SPLITSnow Model



Phase I

Comparisons between Modeled and Measured Radiometric Data

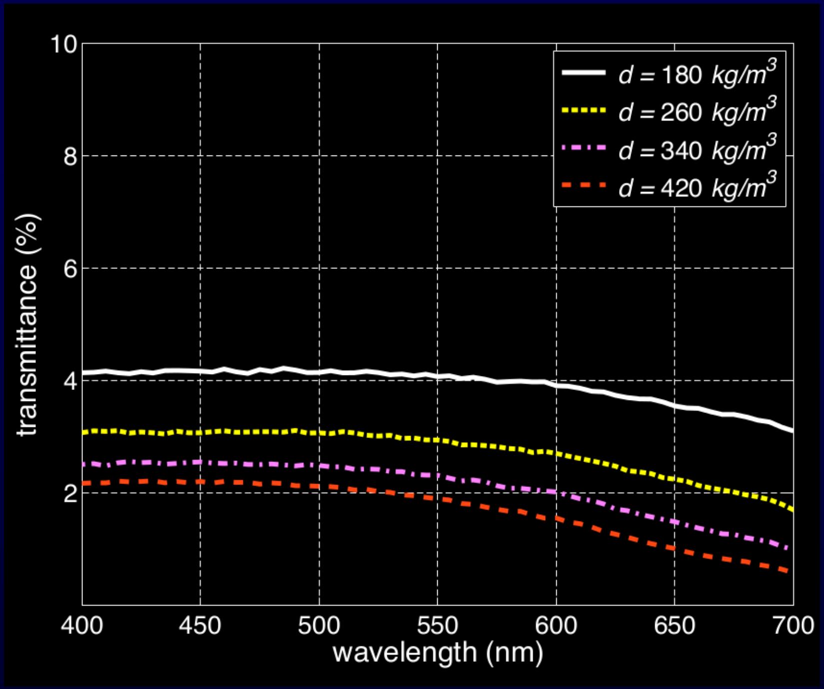
Phase II

Thickness, Saturation, Grain Size and Density Variations

Phase III

Combined Density and Grain Size Variations

➢ Controlled density (*d*) variations



Sample's thickness (depth) equal to 10 cm

- Lower transmittance for denser snow samples: increase of light detour effects
- Consistent with quasi-laboratory findings (Perovich 2007): higher light attenuation for denser snowpacks

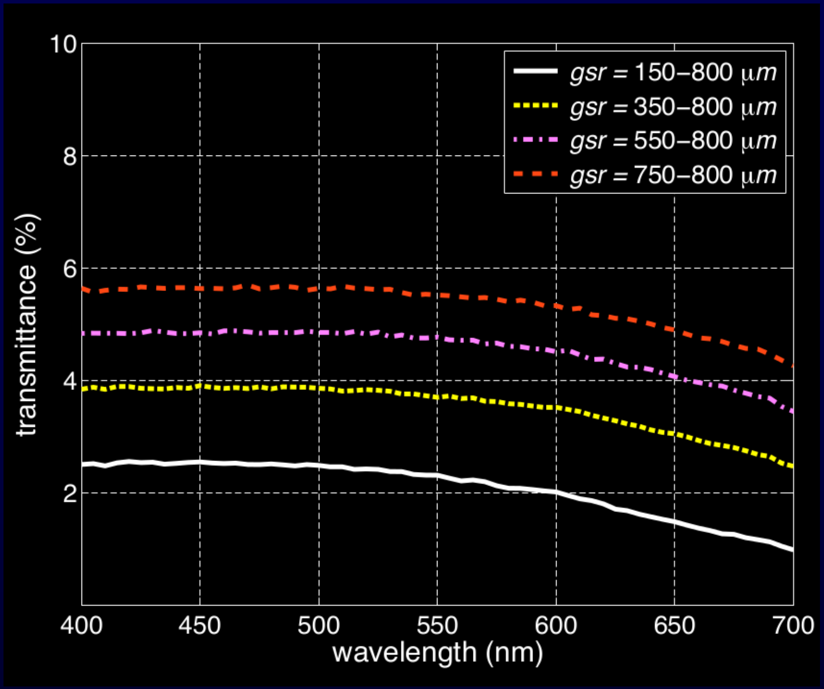
Illustrative Renderings

Low Density

High Density

Distinct thickness values (*e.g.*, 30 cm for the dragon’s main body and 80 cm for the front legs)

➢ Controlled grain size range (*gsr*) variations



Sample's thickness (depth) equal to 10 cm

- Higher transmittance for snow samples with larger grains: larger grains are less likely to scatter light
- Consistent with laboratory experiments involving other particulate materials (*e.g.*, sand-textured soils)

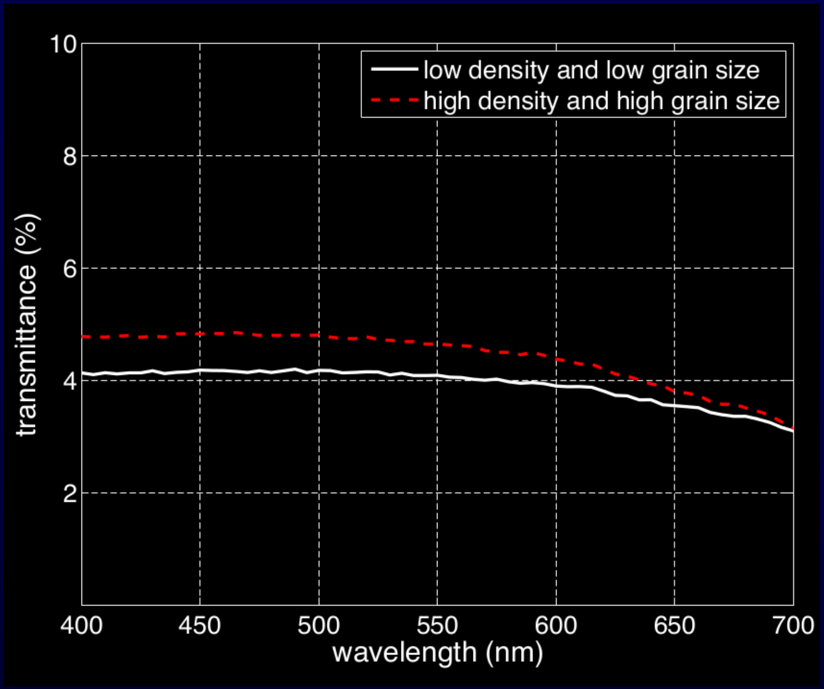
Illustrative Renderings

Low Grain Size

High Grain Size

Distinct thickness values (*e.g.*, 30 cm for the dragon’s main body and 80 cm for the front legs)

➢ Concomitant density and grain size increases



Sample’s thickness (depth) equal to 10 cm

- Higher transmittance
- Consistent with field observations (Gerdel 1941) of snow undergoing metamorphic processes (melting and settling)

Illustrative Renderings

Low Density & Low Grain Size

High Density & High Grain Size

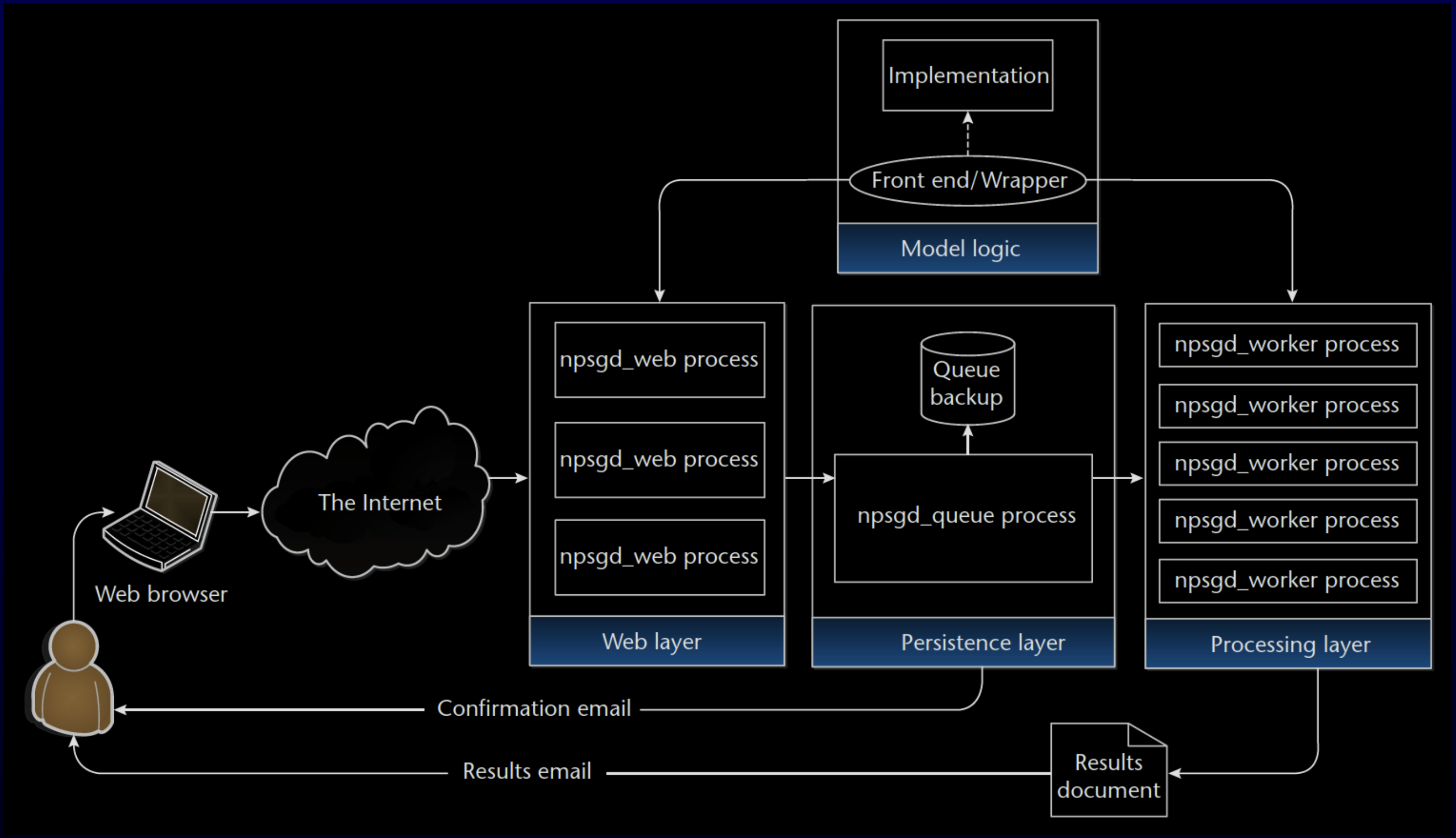
Distinct thickness values (*e.g.*, 30 cm for the dragon's main body and 80 cm for the front legs)

Reproducibility

- Disclosure of the data used in the research to allow the full reproduction of modeled results
  - Parameter values
  - Parameter sources

- Code availability: benefits & risks
  - How about a compromise?

Natural Phenomena Simulation Group Distributed - NPSGD



(Baranoski *et al.*, IEEE Computer Graphics and Applications 2012) npsg.uwaterloo.ca

Natural Phenomena Simulation Group
University of Waterloo

Home | News | Members | Research | Data | Models | Guides | Gallery | Misc. | Contact

ABM-U

Algorithmic BDF Model for Unifacial Plant Leaves

The ABM-U employs an algorithmic Monte Carlo formulation to simulate light interactions with unifacial plant leaves (e.g., corn and sugar cane). More specifically, radiation propagation is treated as a random walk process whose states correspond to the main tissue interfaces found in these leaves. For more details about this model, please refer to our related publications (2006 and 2007). Note that ABM-U provides bidirectional readings. However, one can obtain directional-hemispherical quantities (provided by our online system) by integrating the outgoing light (rays) with respect to the outgoing (collection) hemisphere. Similarly, bihemispherical quantities can be calculated by integrating the bidirectional scattering distribution function (BSDF, or simply BDF) values with respect to incident and collection hemispheres.

The default parameters (on the right) correspond to measured and estimated values for a corn (maize) leaf. The spectral input data files used by the online ABM-U model are available here.

For inquiries regarding this model's usage, please contact us via email.

---

* *The code for this version was last updated and compiled on October 2016.*

Run ABM-U Online

Enter your email address:
(used to send the results)

Model Parameter	Value
Number of samples	100000
Wavelength range	400-2500 nm
Angle of incidence	8 degrees
Surface of incidence	Adaxial
Leaf thickness	0.0204 cm
Mesophyll percentage	80 %
Chlorophyll A concentration	0.0029 g/cm^3
Chlorophyll B concentration	0.0008 g/cm^3
Carotenoids concentration	0.00066 g/cm^3
Protein concentration	0.05793 g/cm^3
Cellulose concentration	0.05804 g/cm^3
Lignin concentration	0.00661 g/cm^3
Cuticle undulations aspect ratio	10
Epidermis cell caps aspect ratio	5
Spongy cell caps aspect ratio	5
Simulate sieve effects	☑

Submit

Created using npsgd.

- In short, despite their risks and costs, reproducibility efforts are essential for:
  - tracking down errors and “bugs”
  - consolidating research contributions
  - enabling the full dissemination of scientific works
  - paving the way for future advances

Schedule

- ✓ Introduction
- ✓ Biophysical Background
- ✓ Drawing Board
- ✓ Data Availability and Quality

Break

- ✓ Design Issues
- ✓ Evaluation Approaches
- ✓ Interdisciplinary Applications
- ❑ Conclusion

Conclusion

➢ Is the rationale behind the *in silico* investigation of open questions about biophysical phenomena something new?

"Science is only useful if it tells you about some experiment that has not been done; it is no good if it only tells you what just went on."

R.P. Feynman
The Character of Physical Law, 1964

- Viewed in this context, a predictive *in silico* experimental framework can also be used to:

  - simulate the behavior of a system under various conditions including those that are still open scientific questions

  - drive new investigations (*e.g.*, the study of material appearance changes elicited by environmental stimulli)

- Hence, it can truly be an effective instrument for fruitful interdisciplinary research

➢ Is interdisciplinary research really attainable?

- It requires a substantial amount of professional and personal effort to overcome technical barriers such as:
  - Data availability & quality
  - Terminology issues
  - Unsound generalizations, …
- … and to acquire a comprehensive understanding about the target problem from a biophysical perspective

- How about “subjective” barriers?
  - Intra-departmental
  - Inter-departmental
  - External
    - Conference and journal reviewing committees
    - Scholarship and grant selection committees

- Is it worth the effort?

- Is it worth the effort?

Depends!

- Is it worth the effort?

Depends!

- Perhaps we should ask ourselves …

- Is it worth the effort?

Depends!

- Perhaps we should ask ourselves …

Do we want to be famous or useful?

Credits: Diagrams, Images and Photos

- Tenn Francis Chen
- Petri Varsa
- Bradley Kimmel
- Aravind Krishnaswamy
- Spencer R. Van Leeuwen
- Denise Eng
- Mark Iwanchyshyn
- Boris Kravchenko
- Sung M. Hong
- Thomas Dimson
- Michael Lam
- Daniel Yim
- Tina Carvalho
- NASA (satellite illustrations)
- Wikimedia, notably Kelvin Song (choloroplasts diagram), Kristian Peters (chloroplasts photo) and Jeremy Kemp (phototherapy photo)

Special thanks to:

- J.T. Woolley
- W.A.G. Bruls and J.C. Van der Leun
- F. Imai
- LOPEX team (B. Hosgood *et al.*)
- SISpec team (R. Salzano *et al.*)
- S. Prahl *et al*.,
- S. Jacquemoud *et al.*
- M. Vrhel *et al.*
- F.P. Zscheile *et al.*
- J.F. Bell III *et al.*
- E.M. Nagel *et al.*
- A.N. Yaroslavsky *et al.*
- J.N. Rinker *et al.*
- NASA-JPL AVIRIS-NG team

and many, many others… without their efforts to measure and distribute fundamental data, we could not have developed our models!

The videos mentioned in the tutorial can be found at:

http://www.npsg.uwaterloo.ca/gallery.php

or

https://www.youtube.com/UWNPSG

This concludes the tutorial!

Thanks!