On the Development of Predictive Models of Light Interaction with Organic and Inorganic Materials

Lecture Series

Gladimir V. G. Baranoski

Natural Phenomena Simulation Group

School of Computer Science

University of Waterloo, Canada

National Institute of Informatics -Tokyo - 2012

Schedule of Lectures

- ✓ Predictability: Benefits and Costs
- ❑ Data Collection: Finding the Pieces of Jigsaw Puzzles
- ❑ Model Design: Balancing Reality and Abstraction
- ❑ Evaluation: The Key for Assessing “Real” Contributions
- ❑ Interdisciplinary Applications: Technical and Political Barriers

Data Collection: Finding the Pieces of Jigsaw Puzzles

Lecture 2

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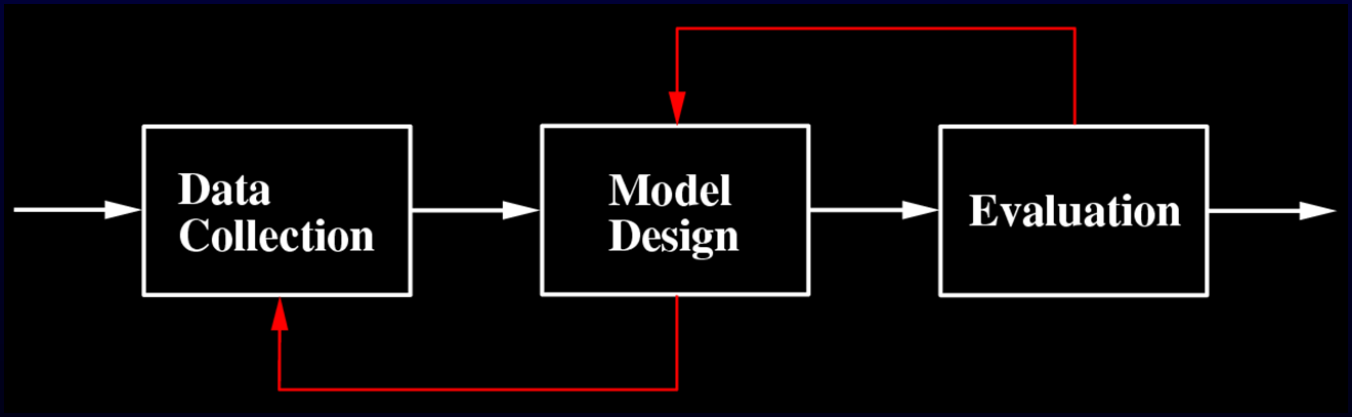
Outline

- What data?
- Biophysical Data Constraints
- Characterization Data Constraints
- Evaluation Data Constraints
- Getting Our Own Data

What data?

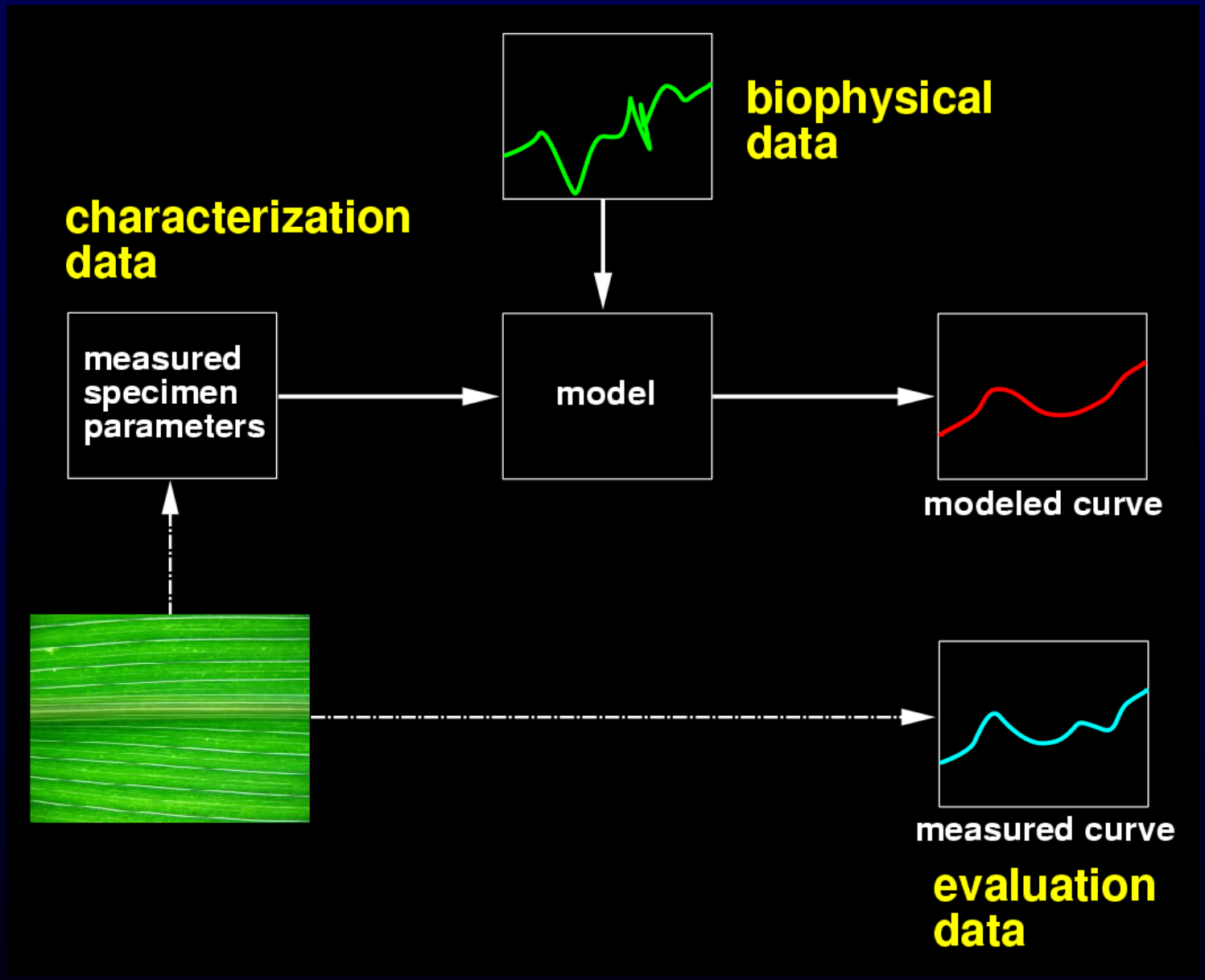
- What are the main steps leading to predictive models?
  - The crossing of field boundaries
  - The use of scientifically sound development frameworks



"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, etc …

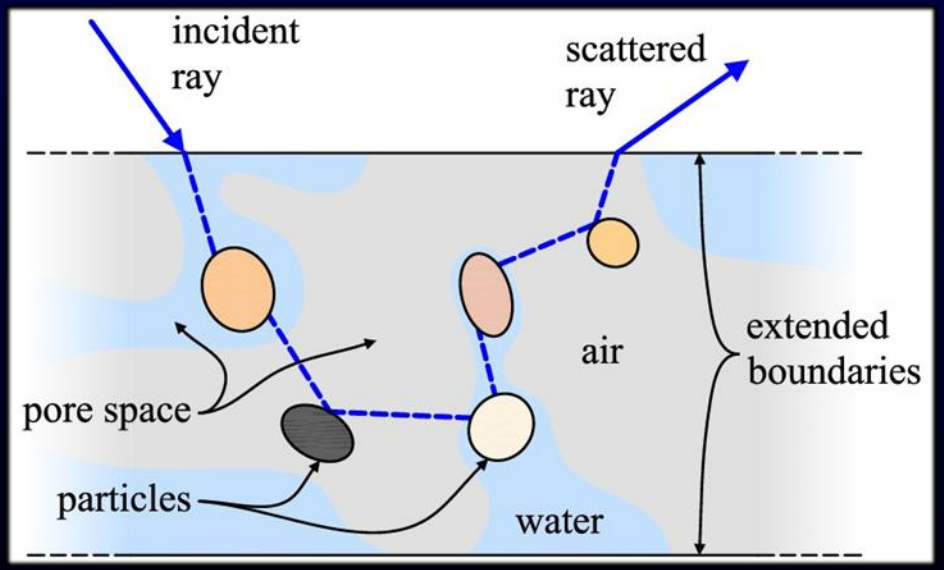

biophysical data
characterization data
measured specimen parameters
model
modeled curve
measured curve
evaluation data

Outline

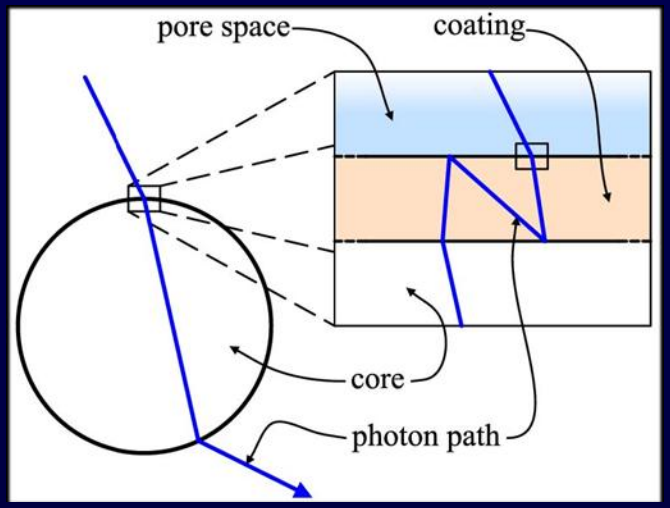
- ✓ What data?
- ❑ Biophysical Data Constraints
- ❑ Characterization Data Constraints
- ❑ Evaluation Data Constraints
- ❑ Getting Our Own Data

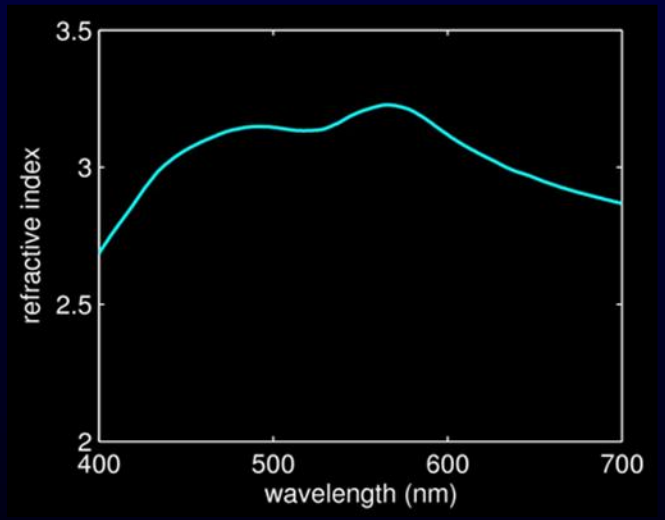
Biophysical Data Constraints

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

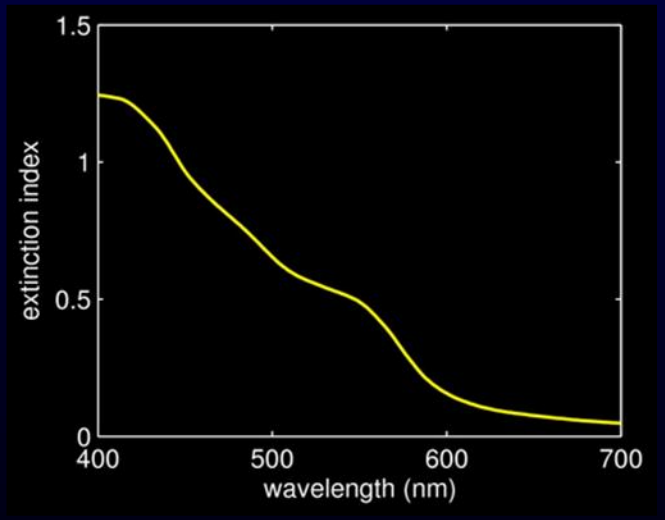


SPLITS





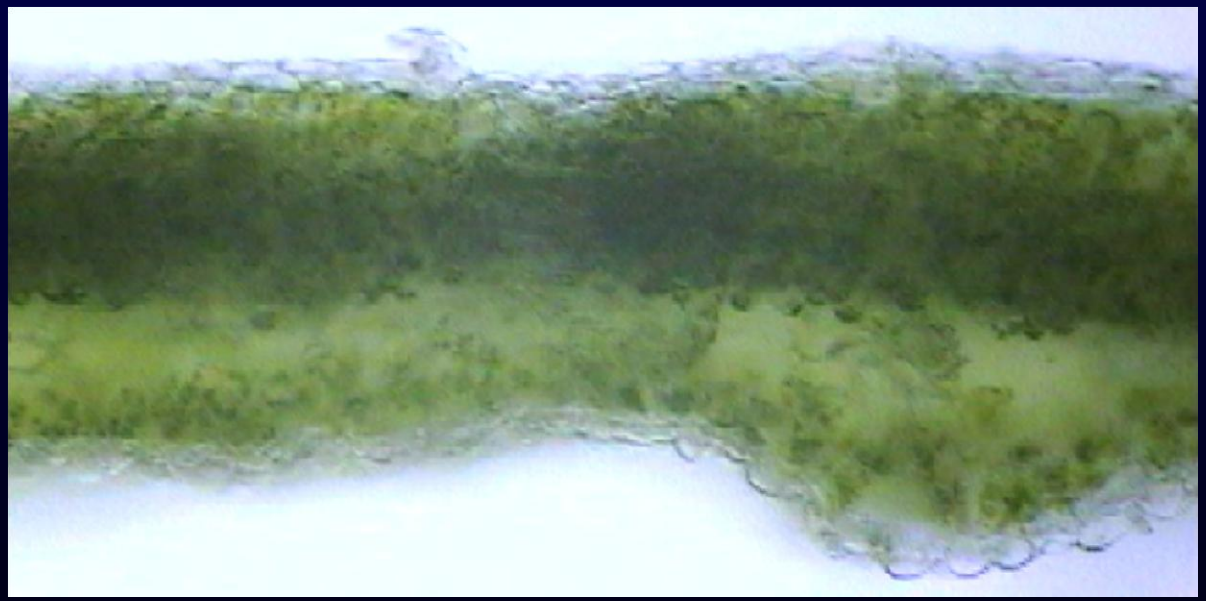
Hematite (red ochre)



- 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:

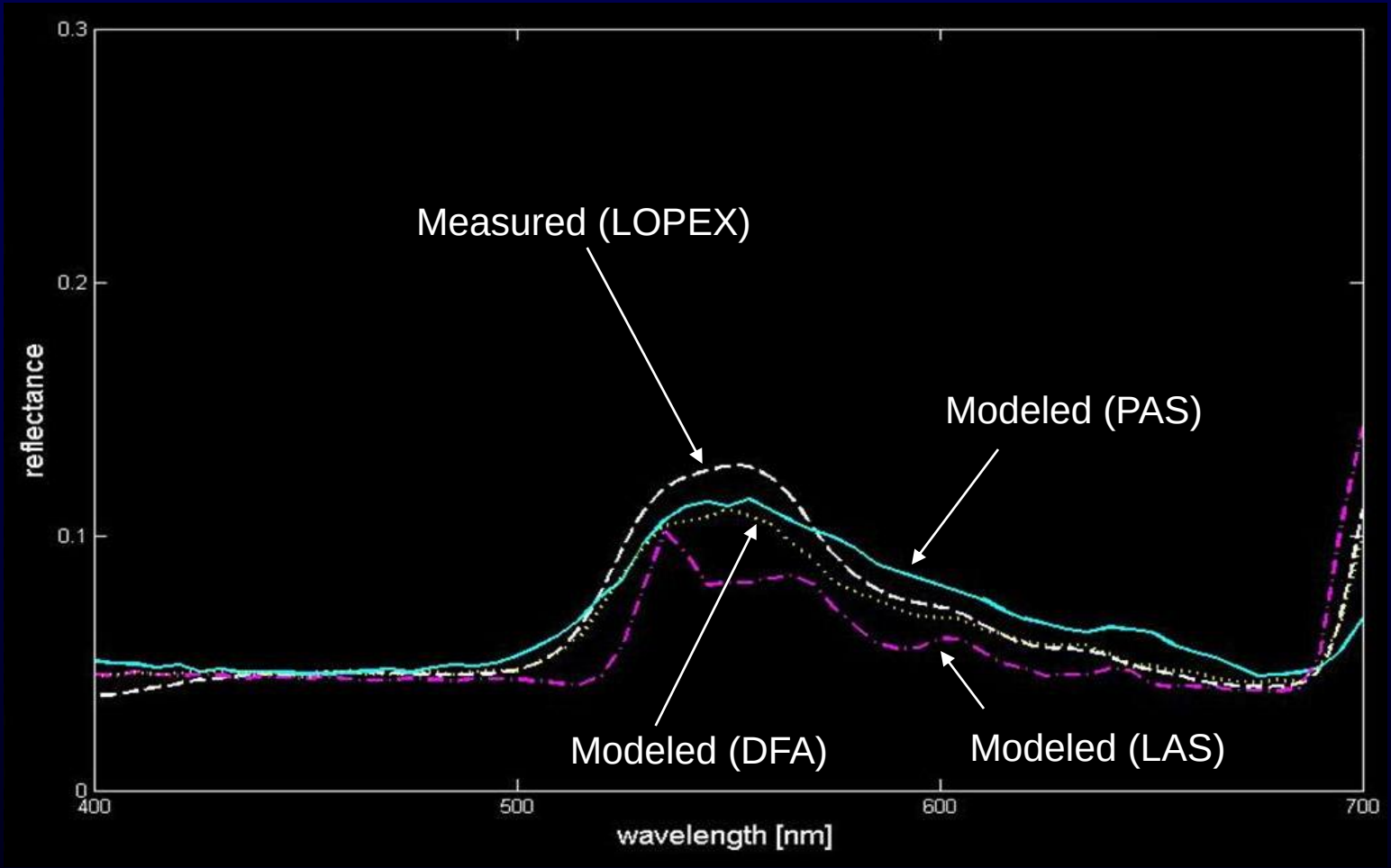
c_s = volume fraction of scatterers,

η_s = refractive index of the scattering material,

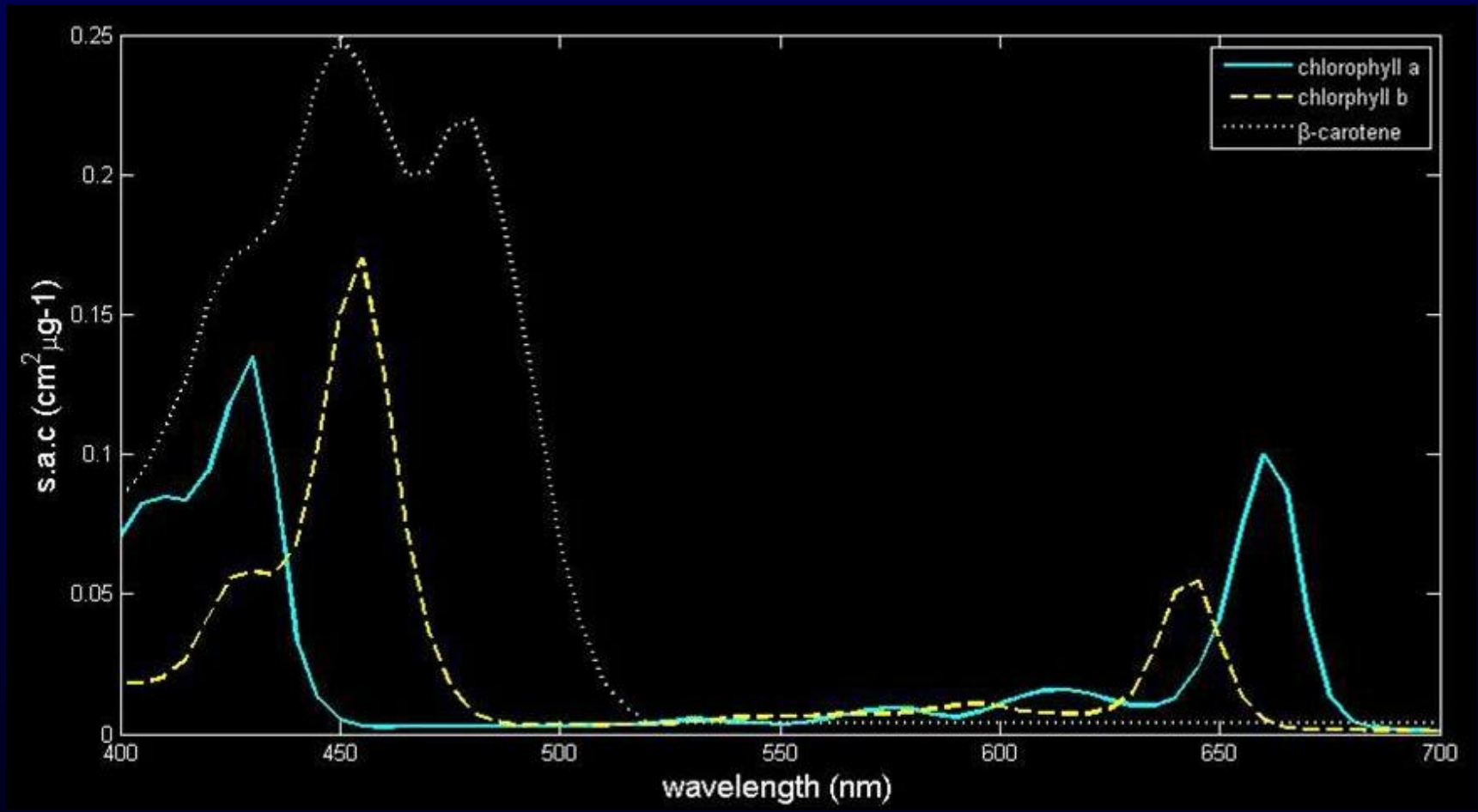
η_b = refractive index of the base material.

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

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

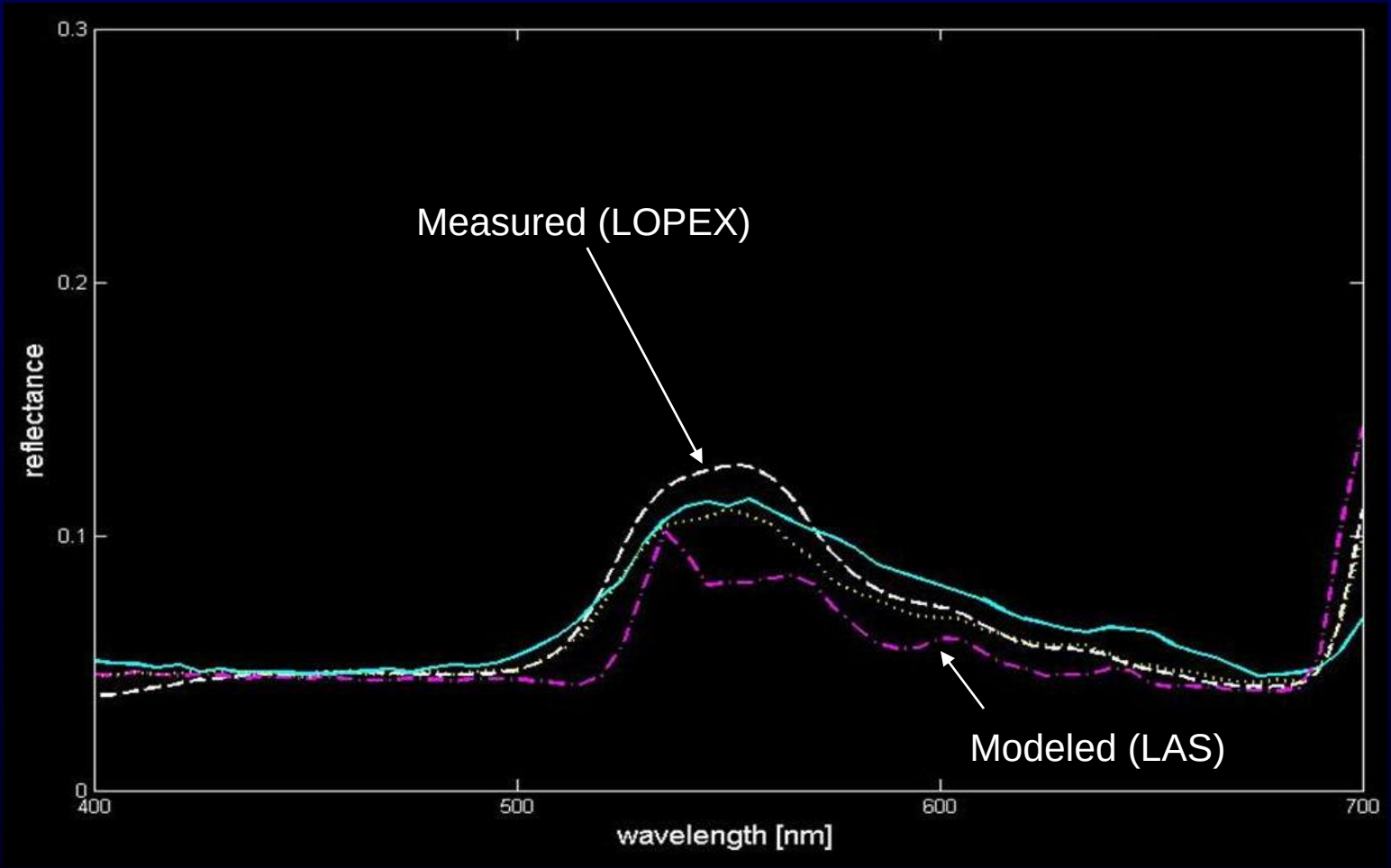


Light Absorption Spectroscopy (LAS)

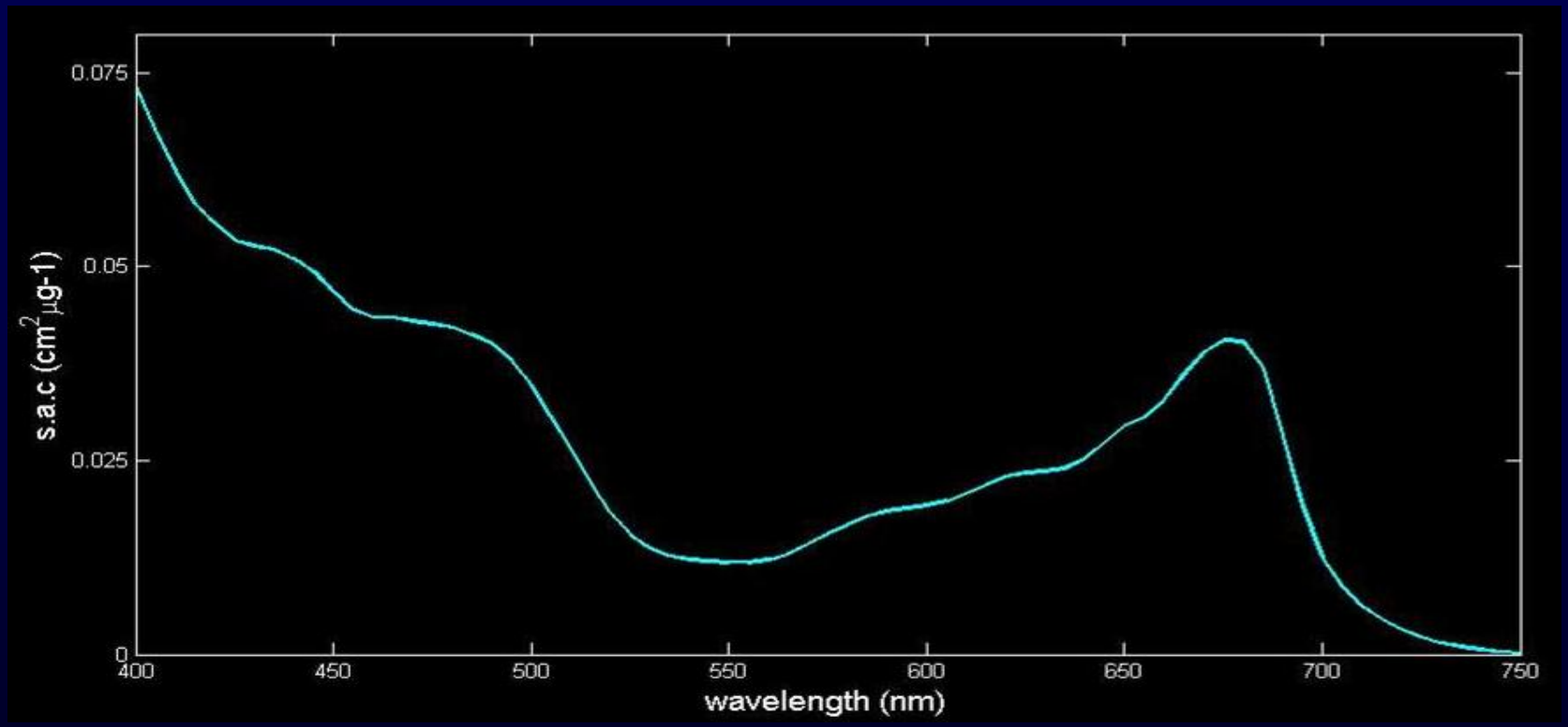


Light Absorption Spectra
(Zscheile and Comar, Botanical Gazette 1941,
Zscheile *et al.*, Plant Physiology 1942)

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

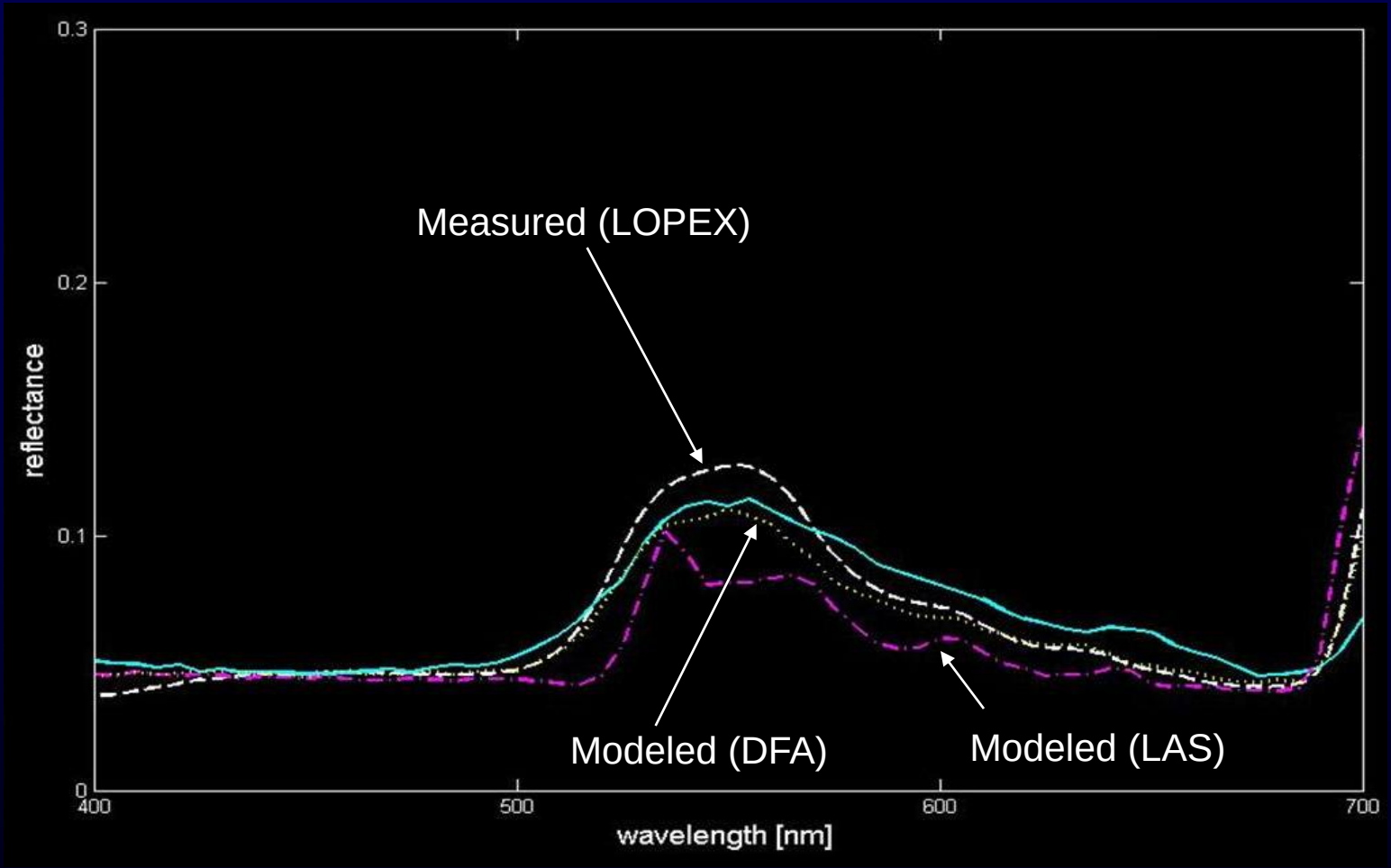


Data Fitting Approach (DFA)

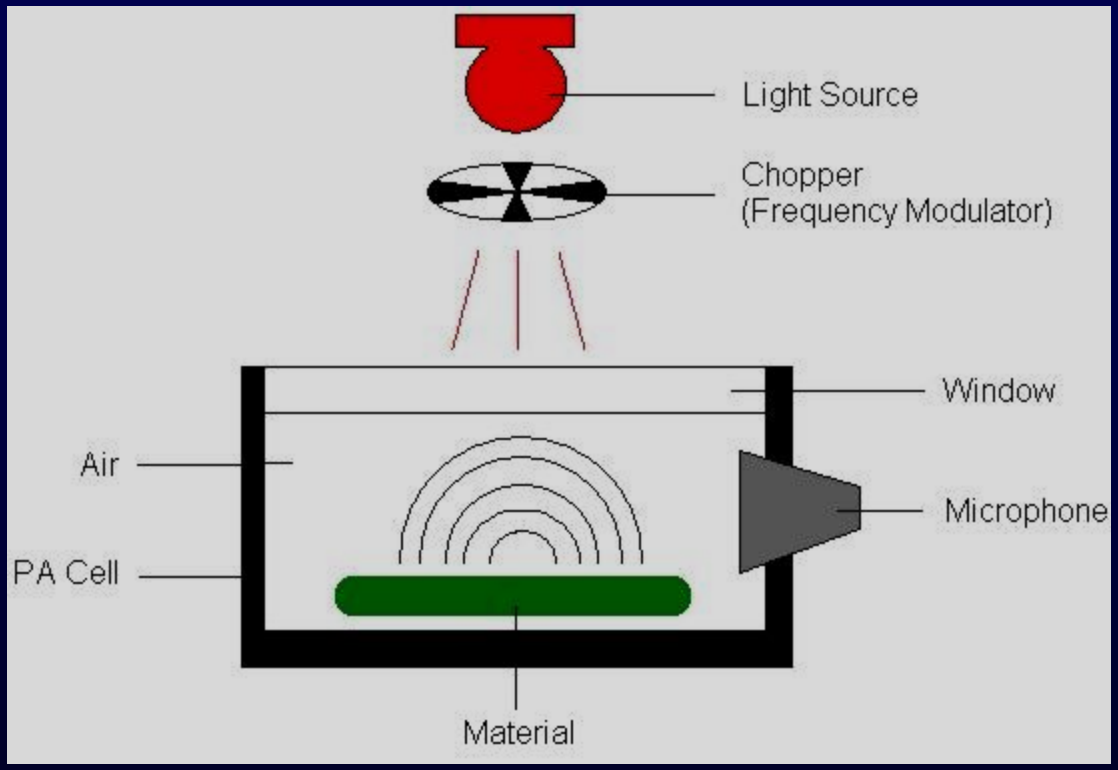


DFA Absorption Spectra for chlorophyll *a+b*
(Jacquemoud *et al.*, Remote Sensing of Environment 1996)

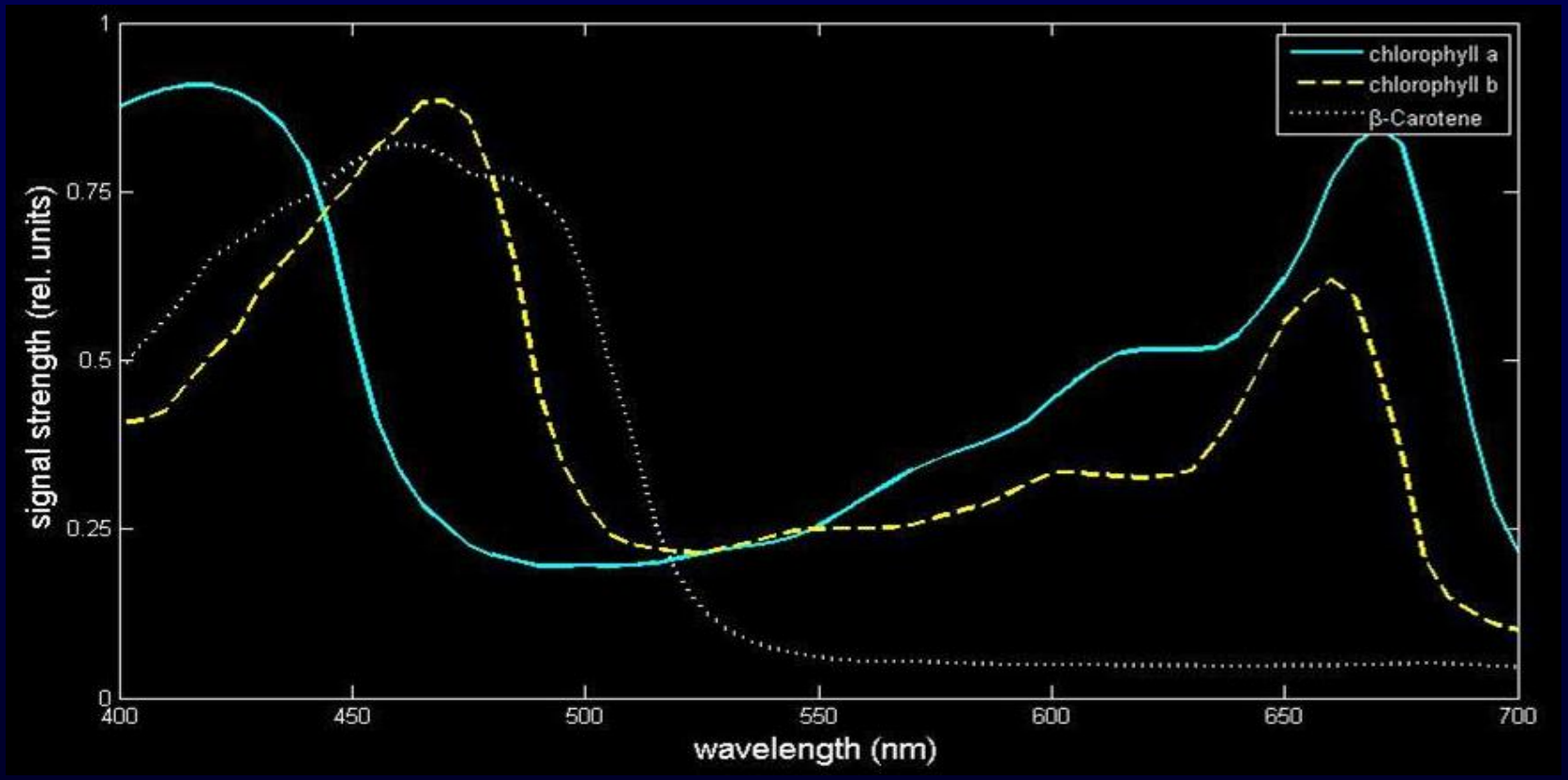
Measured and Modeled (ABM-B) Reflectance Curves of a Soy Leaf



Photoacoustic Absorption Spectroscopy (PAS)

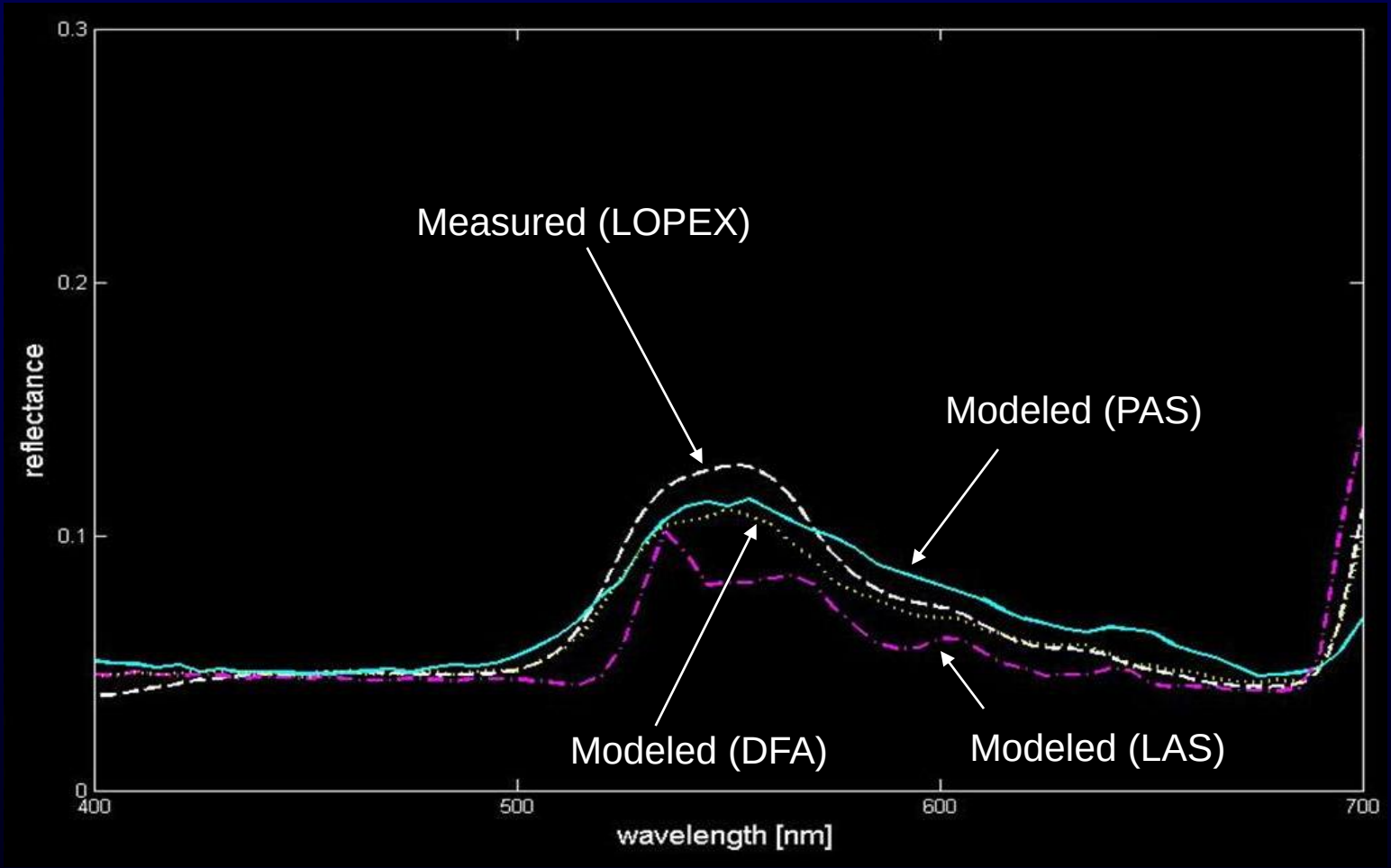


Photoacoustic Spectrometer



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

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



- Remark: same issues apply to the carotenoids ...

❖ … and are worse for tannins and anthocyanins

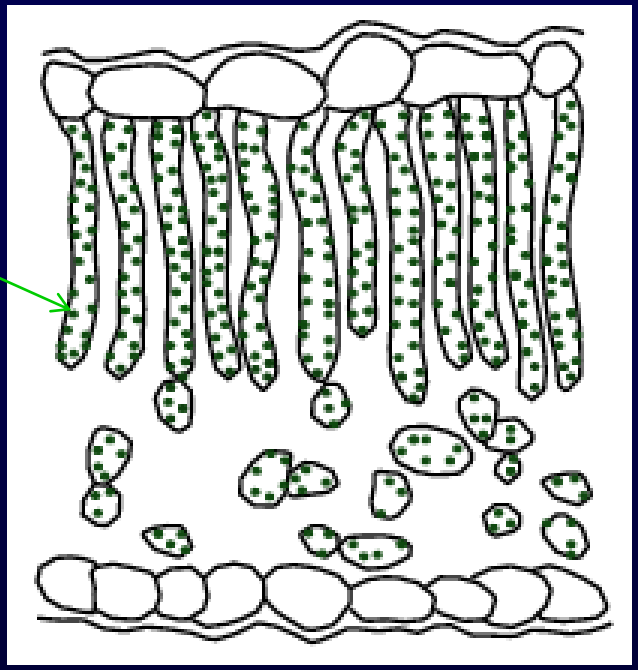
➢ Reliability issues: *in vivo* vs. *in vitro*

→

In vivo
pigments

In vitro
pigments

Cross-Section of a Plant Leaf



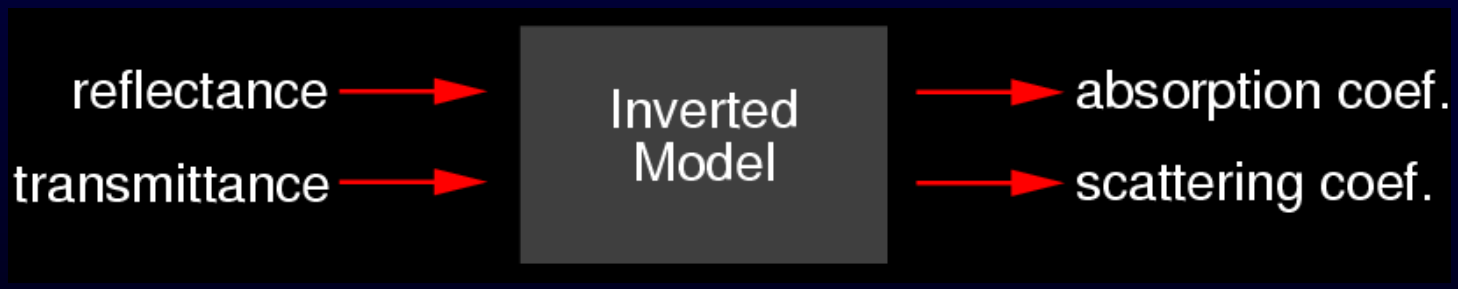
Chlorophyll Solution

- Sieve and detour effects
- Spectral shifts

- Biophysical data derived from inversion procedures

  - Inversion procedure: a way to derive biochemical and optical properties from *in situ* and non-invasive measurements

  - “Inversion” implies a reversal of the usual process of calculating reflection and transmission



Was the model fully evaluated?

Outline

- ✓ What data?
- ✓ Biophysical Data Constraints
- ❑ Characterization Data Constraints
- ❑ Evaluation Data Constraints
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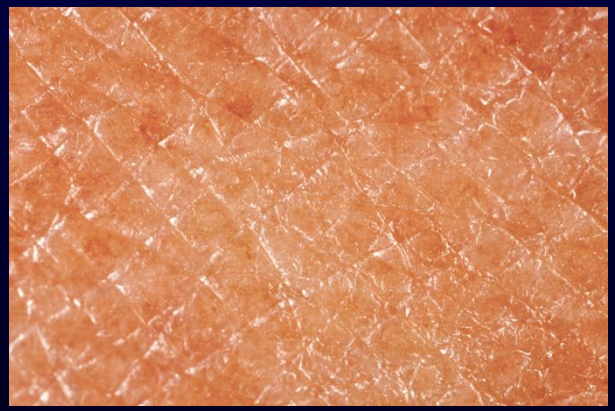
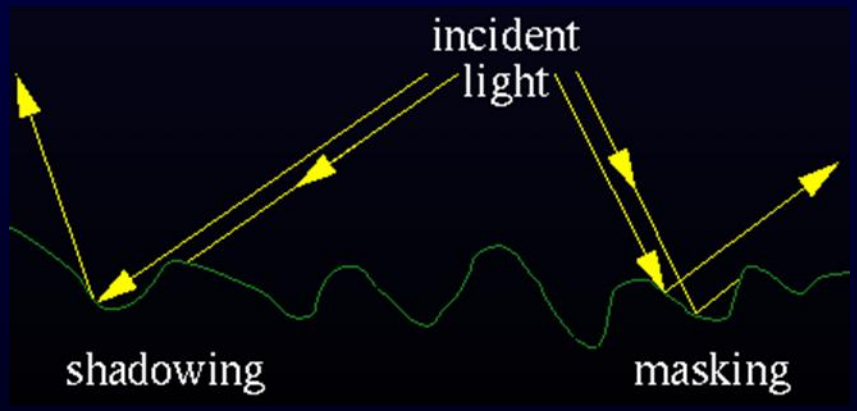
Characterization Data Constraints

- Scarcity
  - Structural parameters affecting light and matter interactions

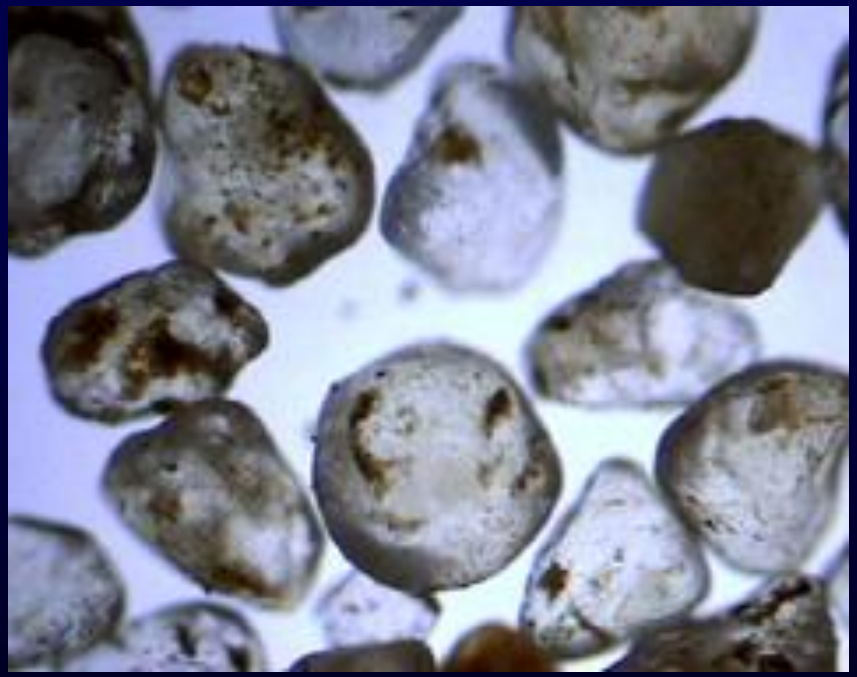
Skin Surface

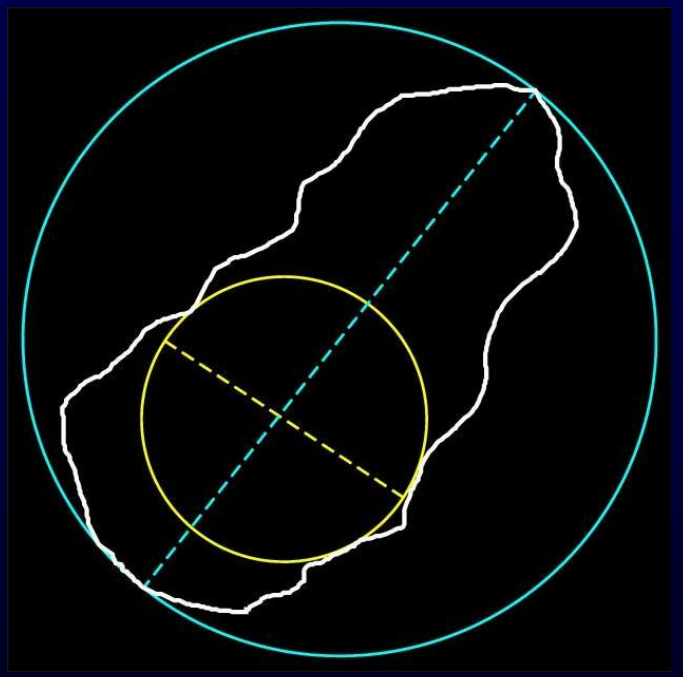




- venation systems and hairs

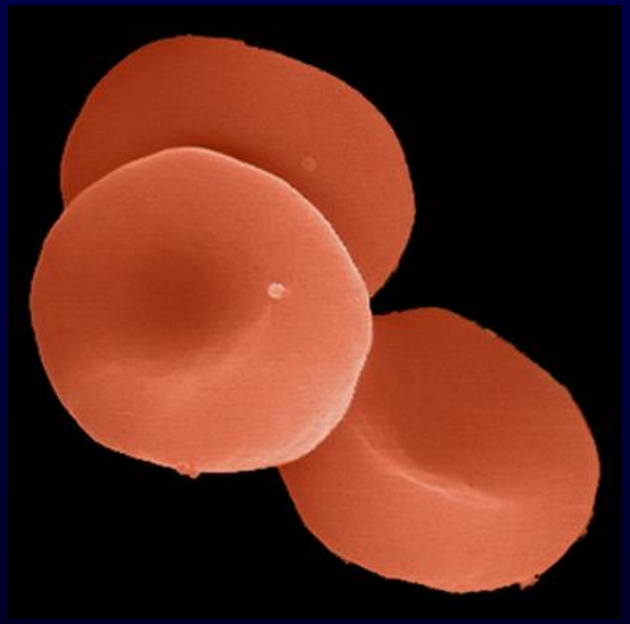
- sand grains (dimensions, shape and roundness)



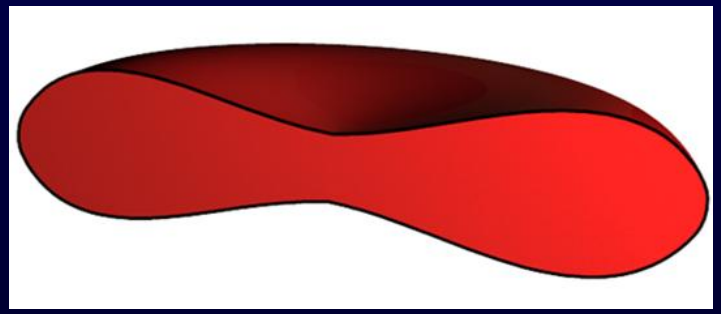


- red blood cells (volume and contour)

RBCs (SEM)

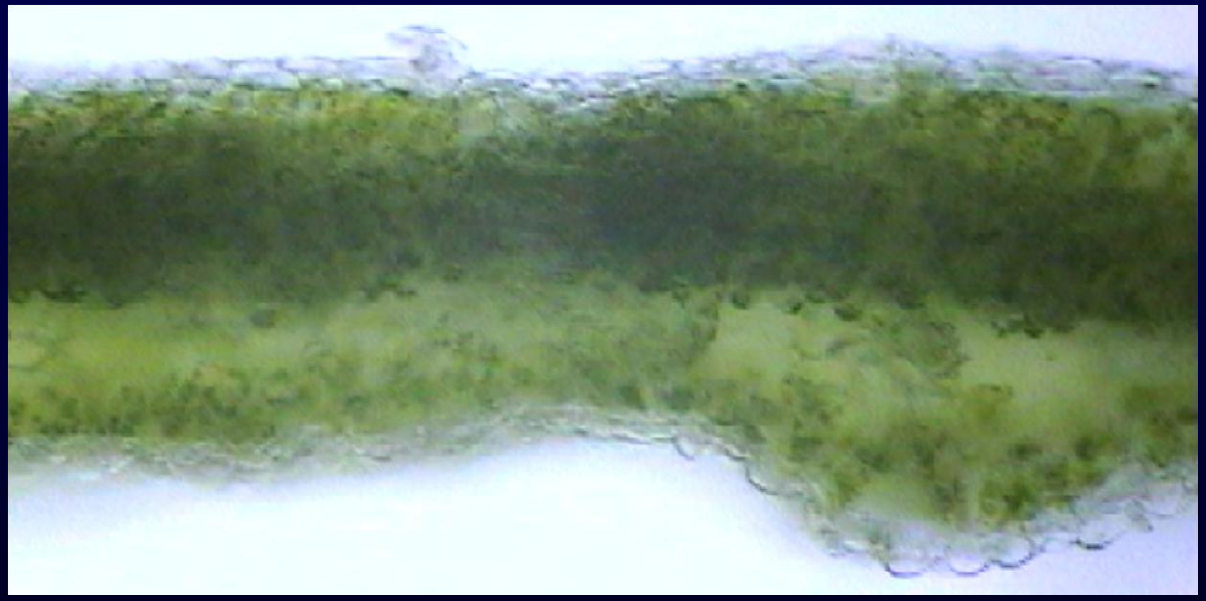


RBC Cross-Section (sketch)

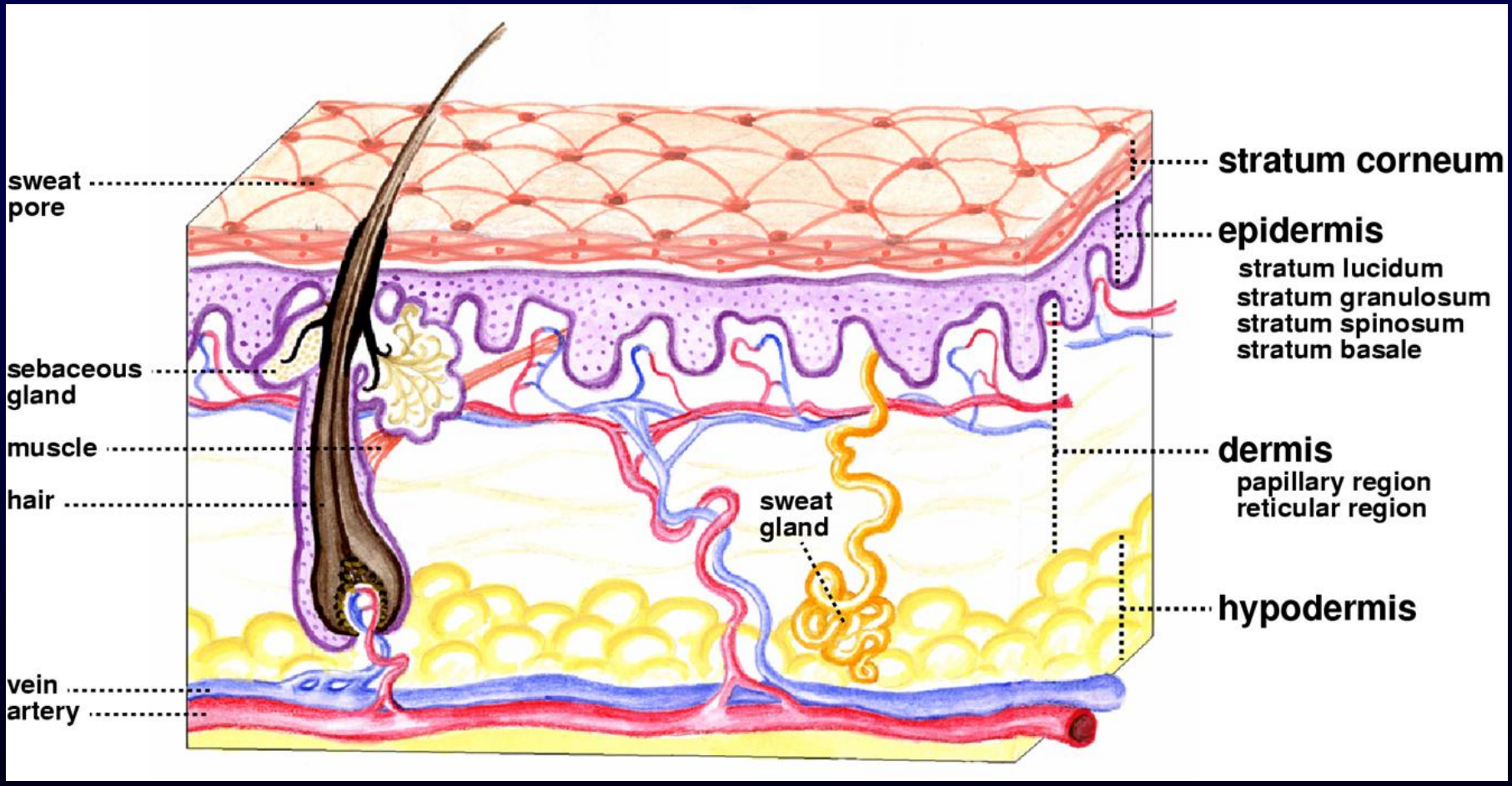


- tissue thickness

Leaf Cross-Section



Human Skin Diagram



- Pigment contents
  - Example: in human skin, light absorption comes mostly from a natural pigment, melanin, found in organelles (melanosomes) inside cells (melanocytes) located in the epidermis

- Melanin is produced by the melanocytes through a photobiological process: melanogenesis

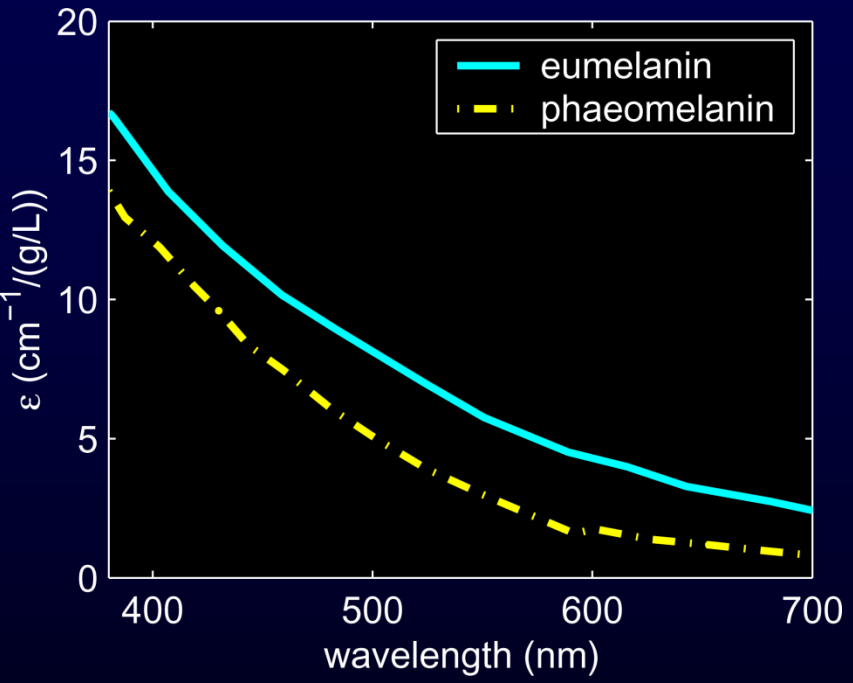
- The amount of melanin produced is determined by both genetic factors and exposure to sunlight (UV)

- Melanin absorption level depends on the number of melanosomes per unit volume

  - *e.g.*, 1.3% for lightly pigmented specimens

  - *e.g.*, 43% for darkly pigmented specimens

- Types of melanin present in the epidermis
  - red/yellow phaeomelanin
  - brown/back eumelanin

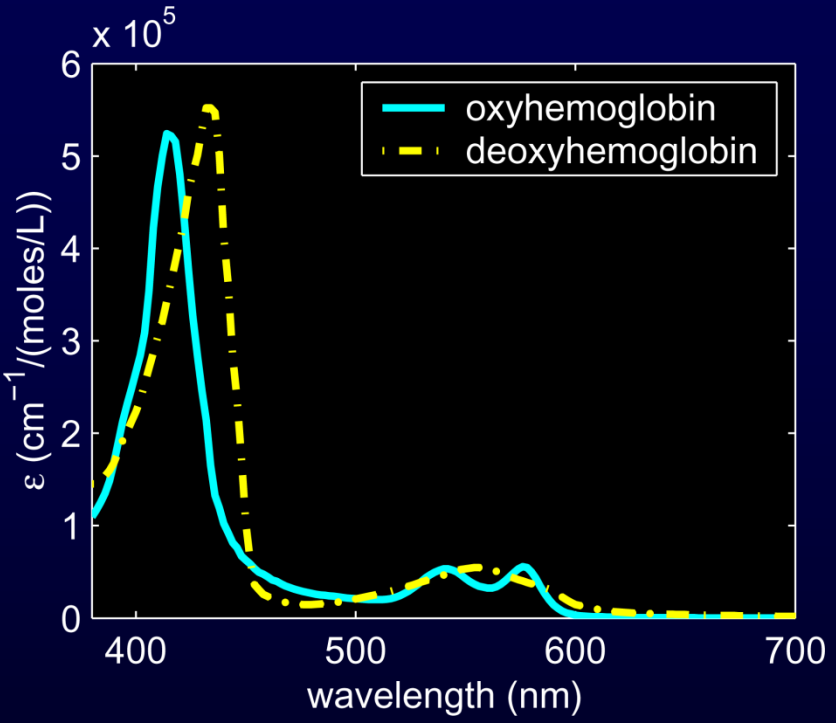


(Jacques, Tech. Rep. OMLC 2001)

- β-carotene is also present in the epidermis

- The dermis layer can be divided into two main layers:
  - ❖ the papillary dermis (smaller blood vessels)
  - ❖ the reticular dermis (larger blood vessels)
- Absorption comes from blood borne pigments:
  - ❖ hemoglobin, bilirubin and β-carotene

- The two types of hemoglobin (oxygenated and deoxygenated) give blood its reddish color



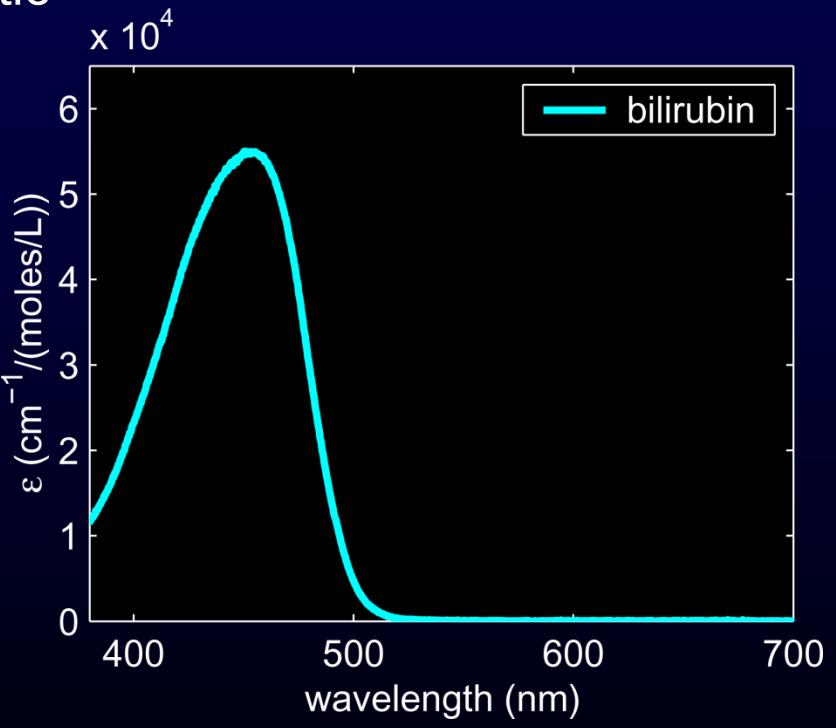
(Prahl, Tech. Rep. OMLC 1999)

- Volume fraction of blood in the dermal tissues can vary roughly in the range 0.2-7% range

- Bilirubin

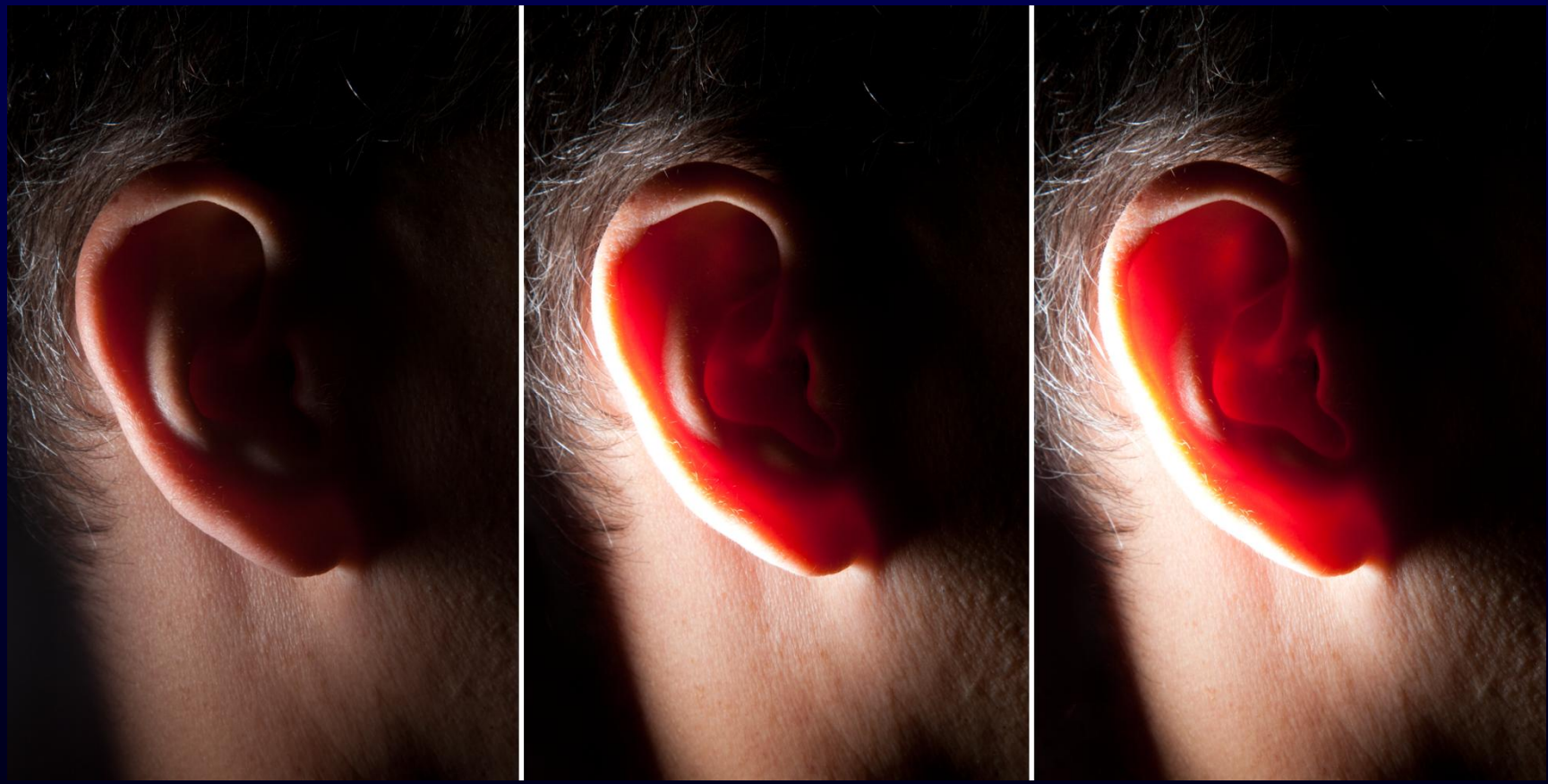
  - an orange-yellow pigment derived from the degradation of hemoglobin during the normal and abnormal destruction of red blood cells

  - excessive amounts in the characteristic jaundice (yellowish) appearance



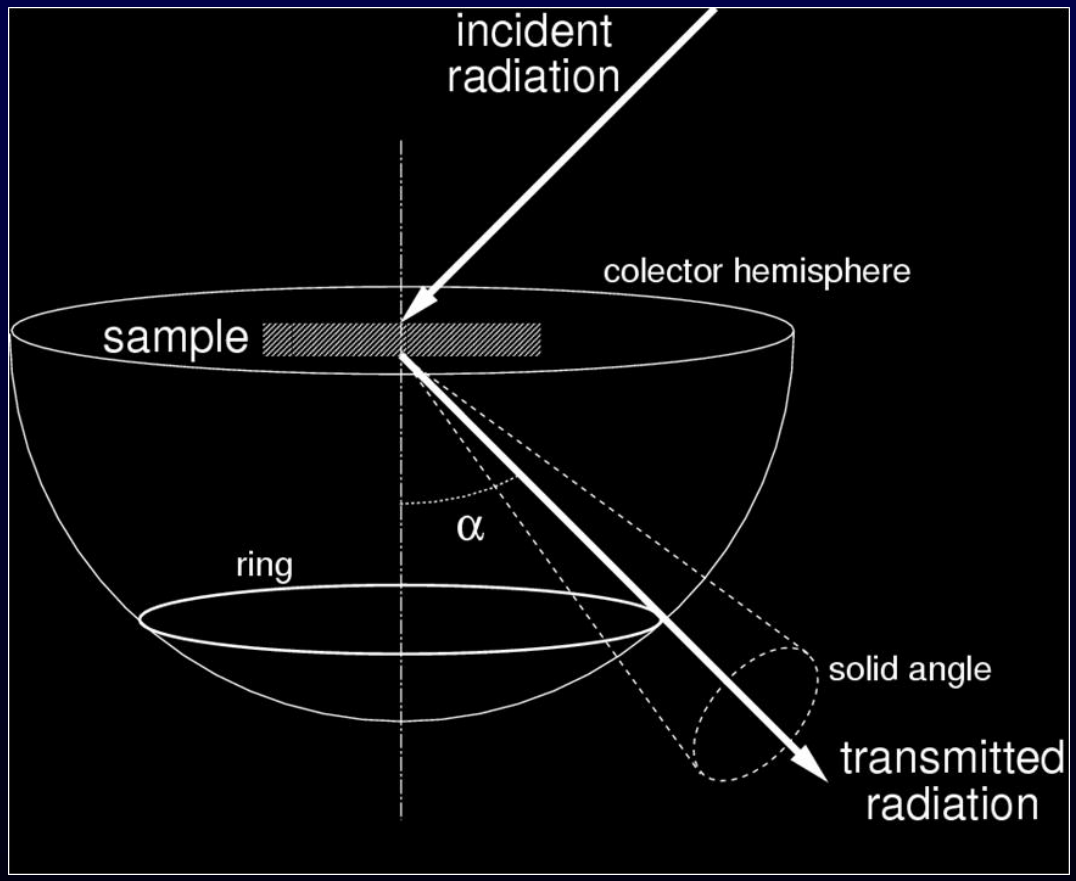
(Prahl, Tech. Rep. OMLC 2001)

- Subsurface scattering data

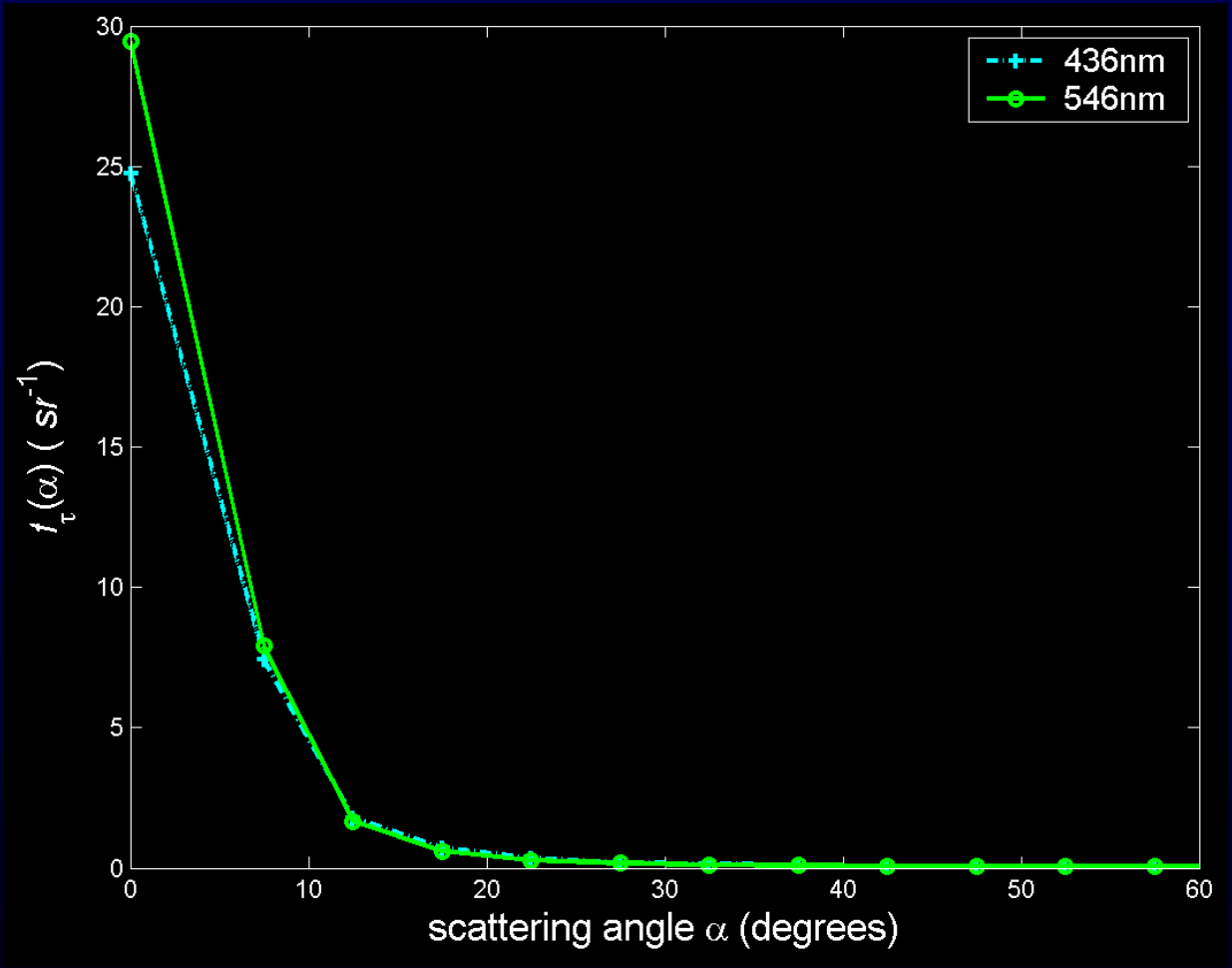


- Scattering data is usually limited to a few wavelengths

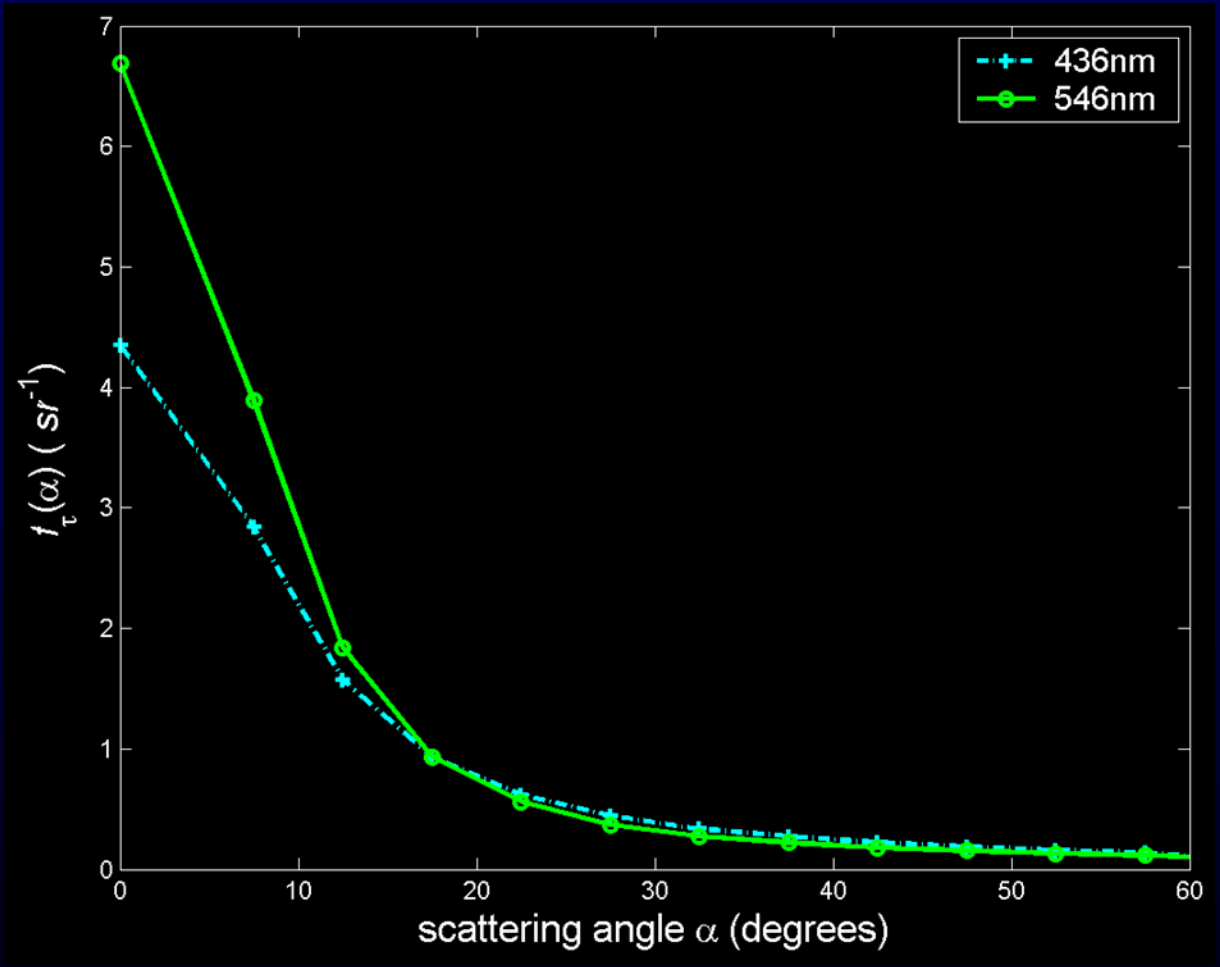
  - Example: skin subsurface measurements performed by Bruls and van der Leun (1984)



❖ Stratum corneum



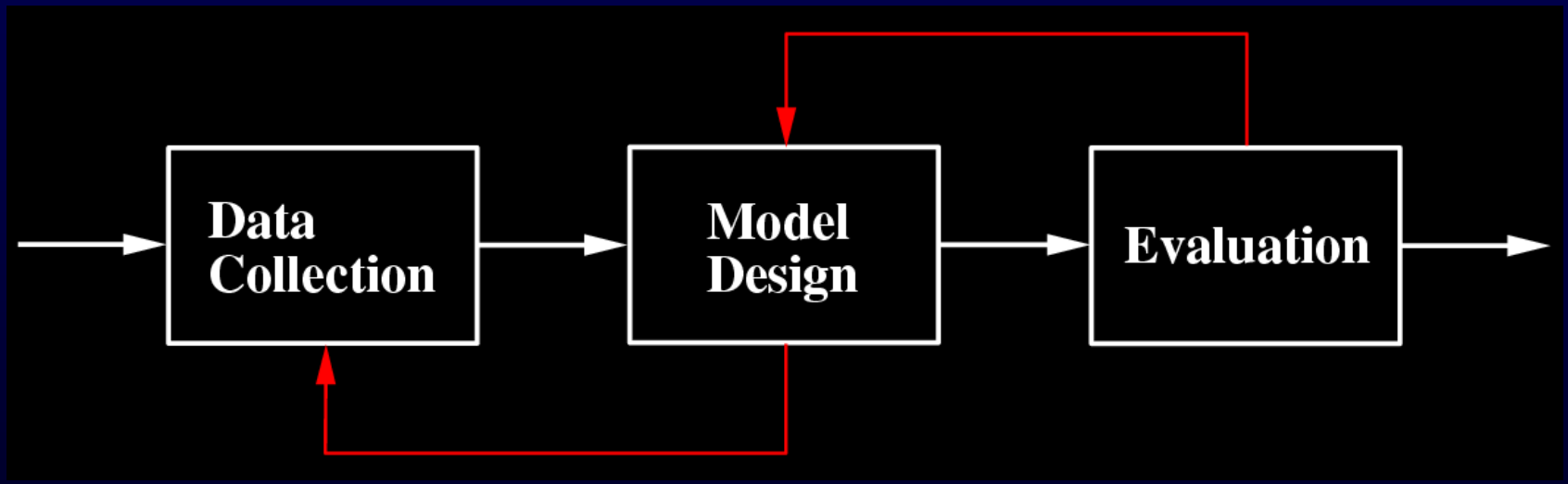
❖ Epidermis

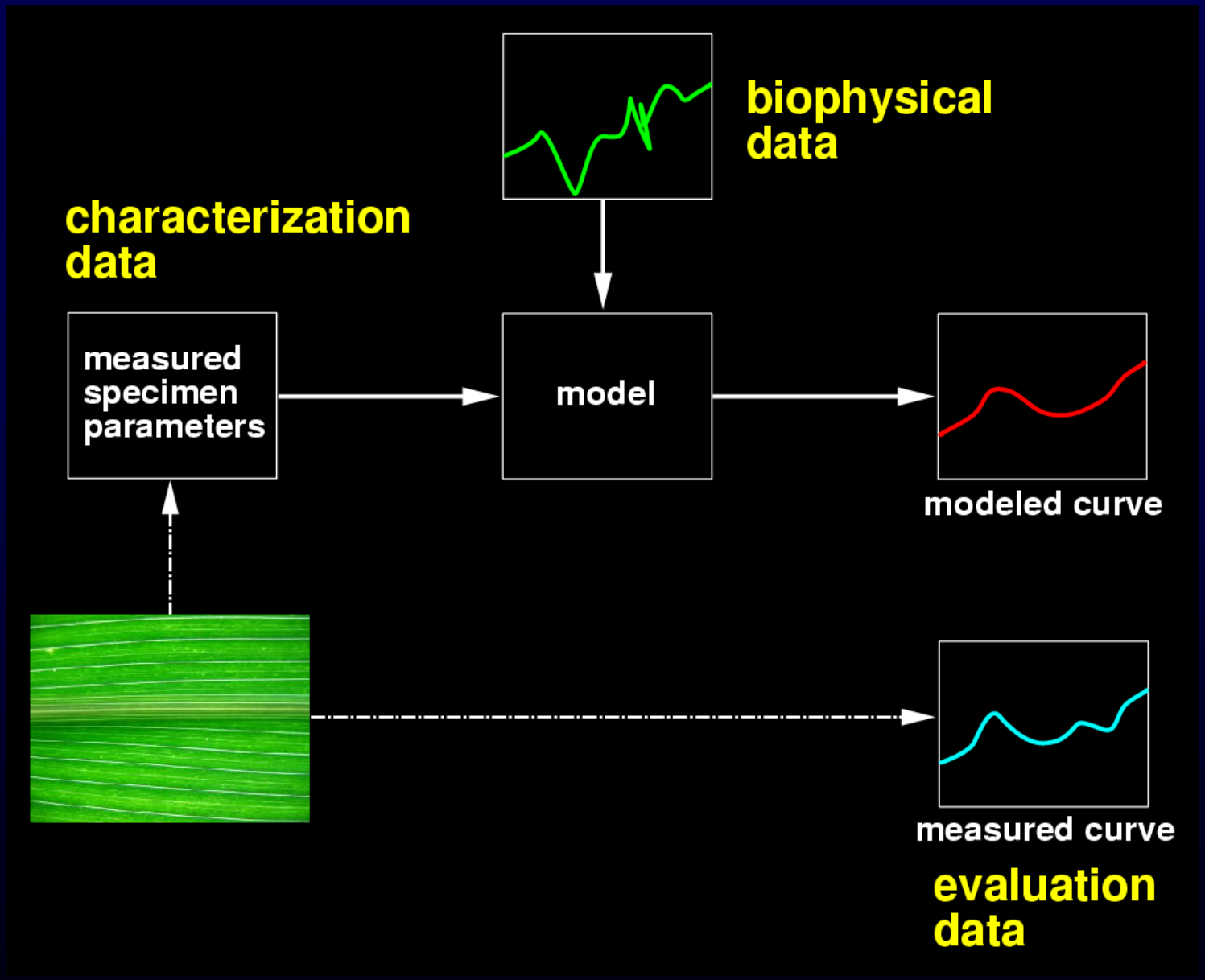

436nm
546nm
$f_\tau(\alpha)$ (sr^{-1})
scattering angle α (degrees)
0
1
2
3
4
5
6
7
0
10
20
30
40
50
60

Outline

- ✓ What data?
- ✓ Biophysical Data Constraints
- ✓ Characterization Data Constraints
- ❑ Evaluation Data Constraints
- ❑ Getting Our Own Data

Evaluation Data Constraints




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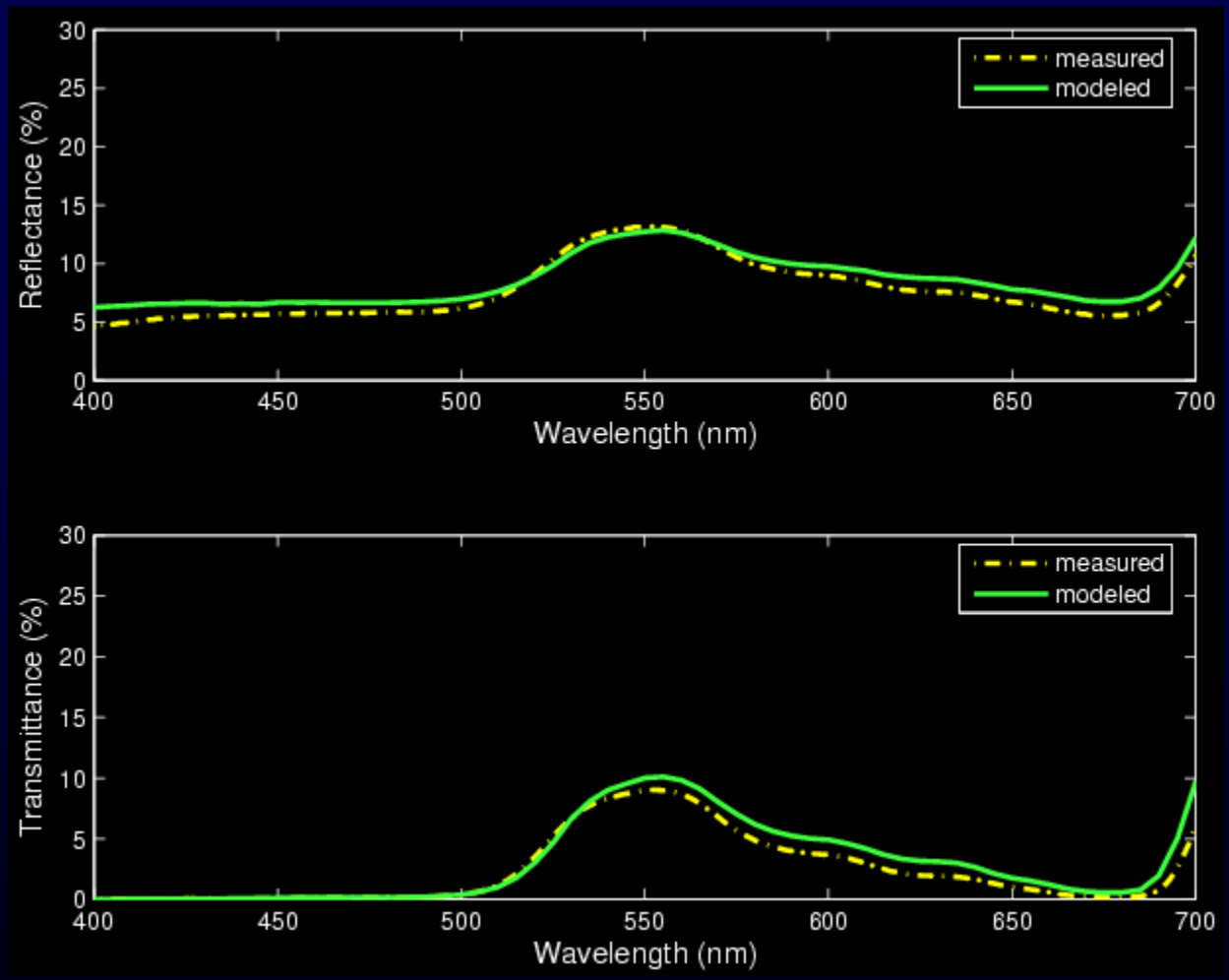
evaluation data

➢ Scarcity

- Spectral databases rarely include the specimen's characterization data
  - Noteworthy example: Leaf Optical Experiments 1993 (LOPEX'93)
    - ❖ thickness
    - ❖ fresh and dry weights
    - ❖ concentration of absorbers (chlorophylls, carotenoids, cellulose, lignin and protein)

Reflectance Curves of a Corn Leaf



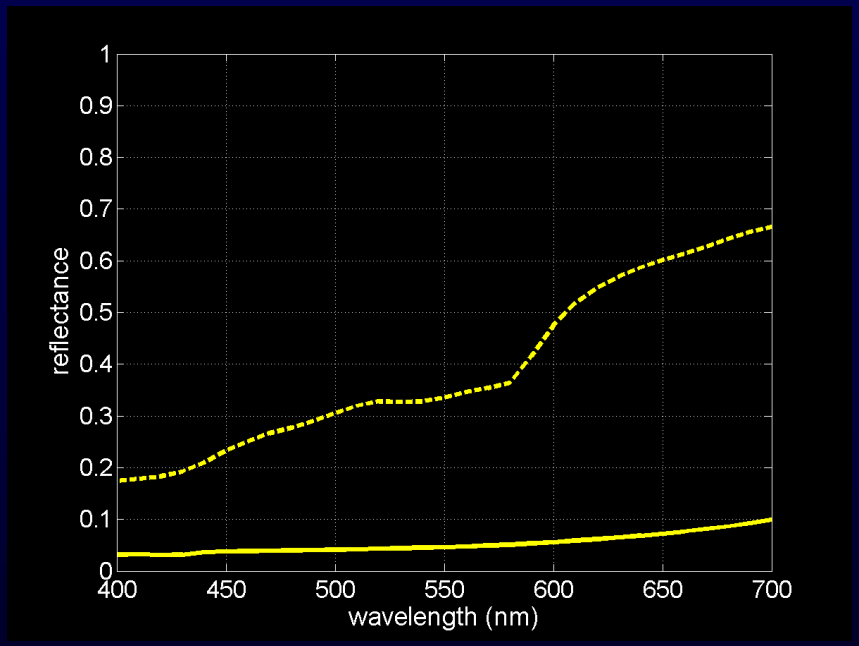
LOPEX

ABM-U

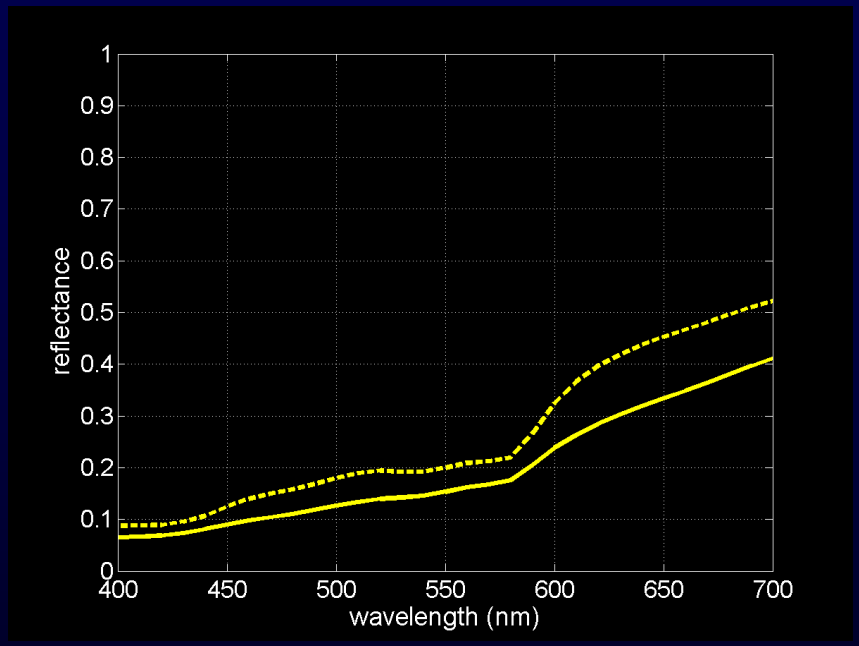
➢ Qualitative descriptions

- How these descriptions really relate to material parameters?
  - Example: human subjects and pigmentation
    - ❖ African
    - ❖ Caucasian
    - ❖ Indian
    - ❖ Asian

African

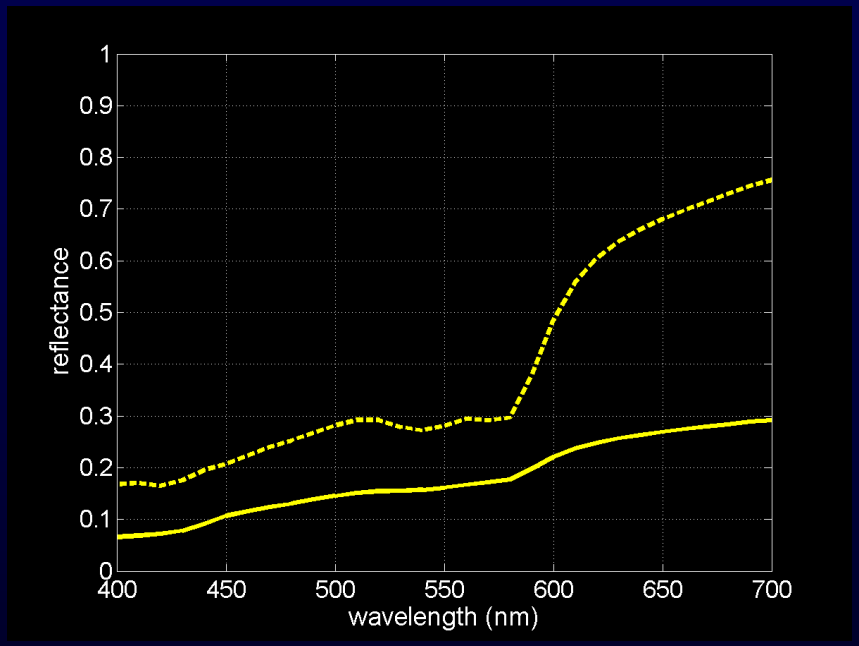


Indian

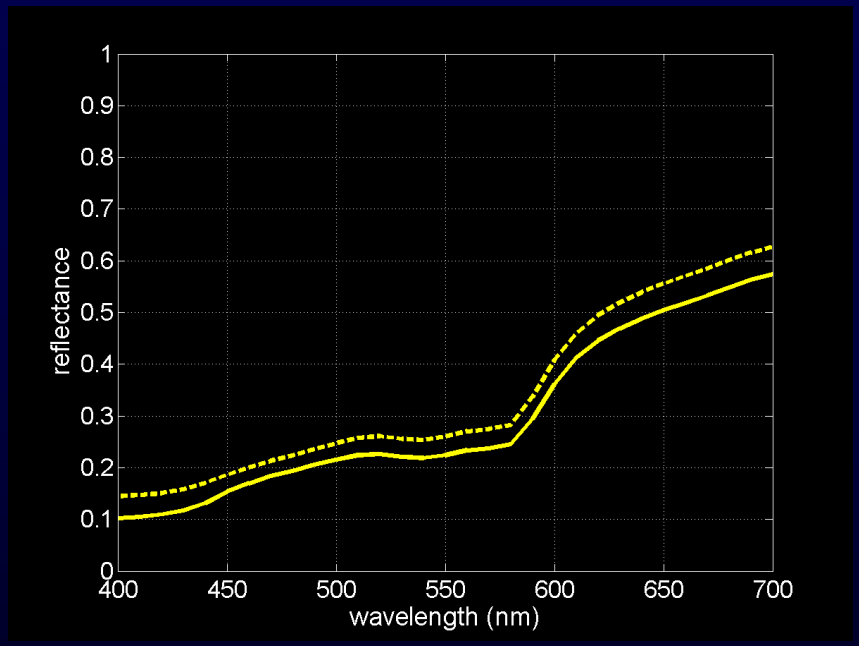


(Vrhel *et al.*, Color Res. Appl. 1994)

Caucasian



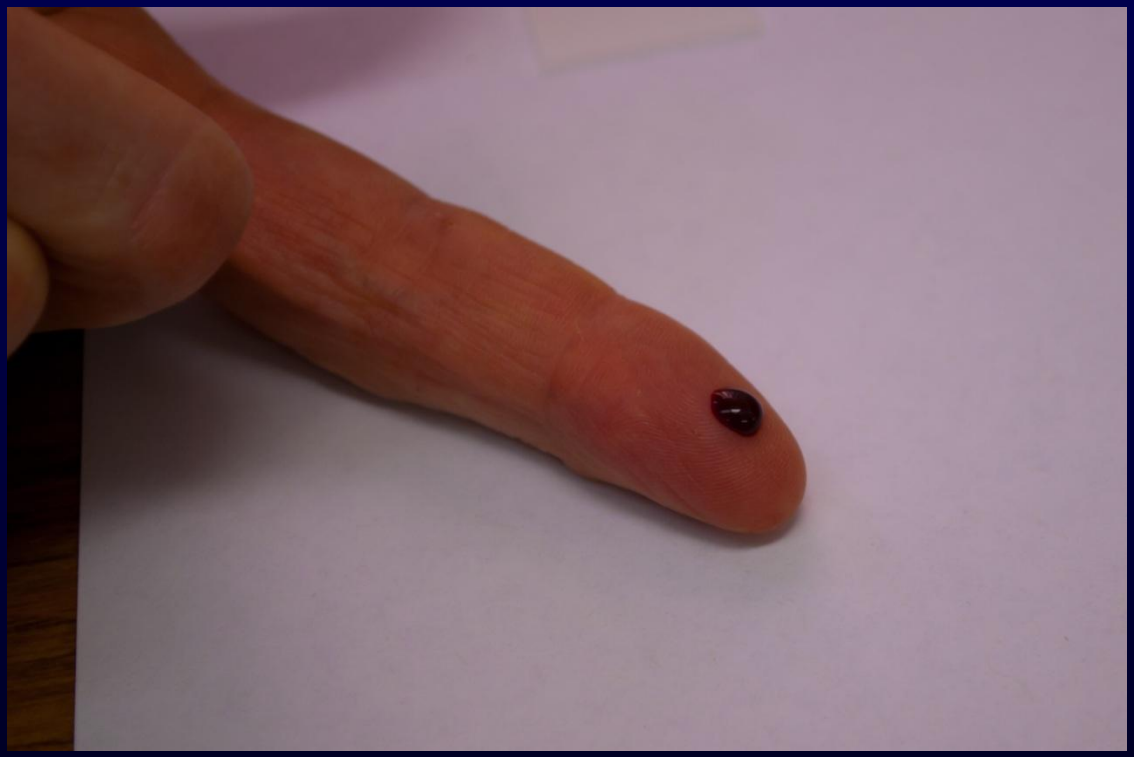
Asian



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

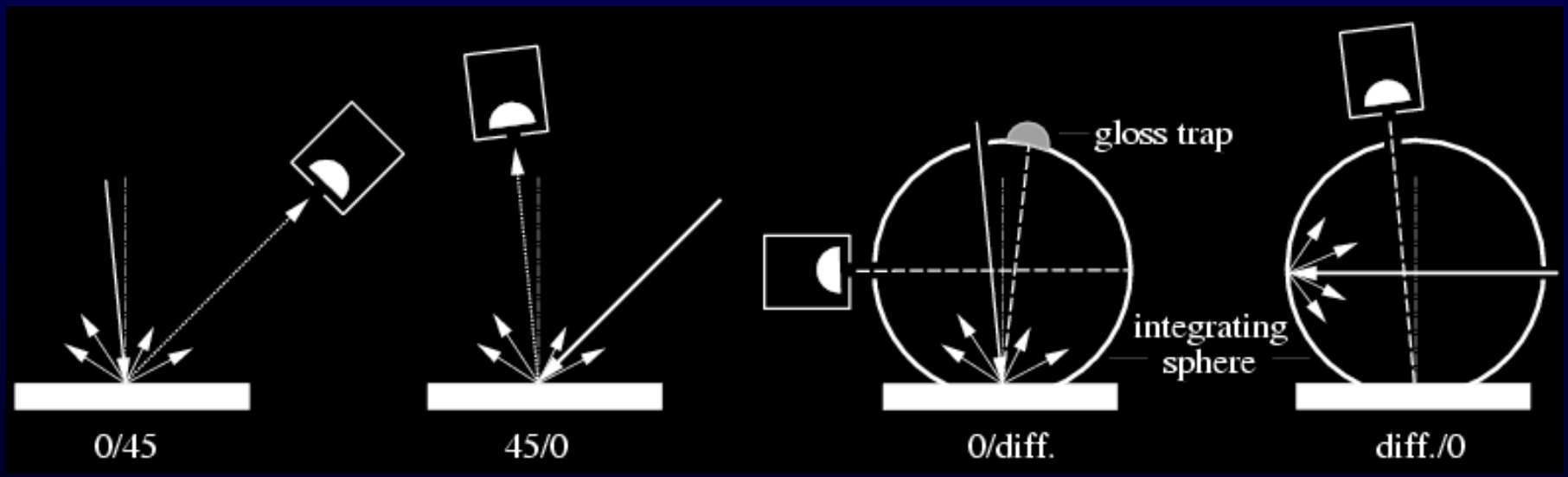
How about tanned specimens?

How about blood flow conditions?

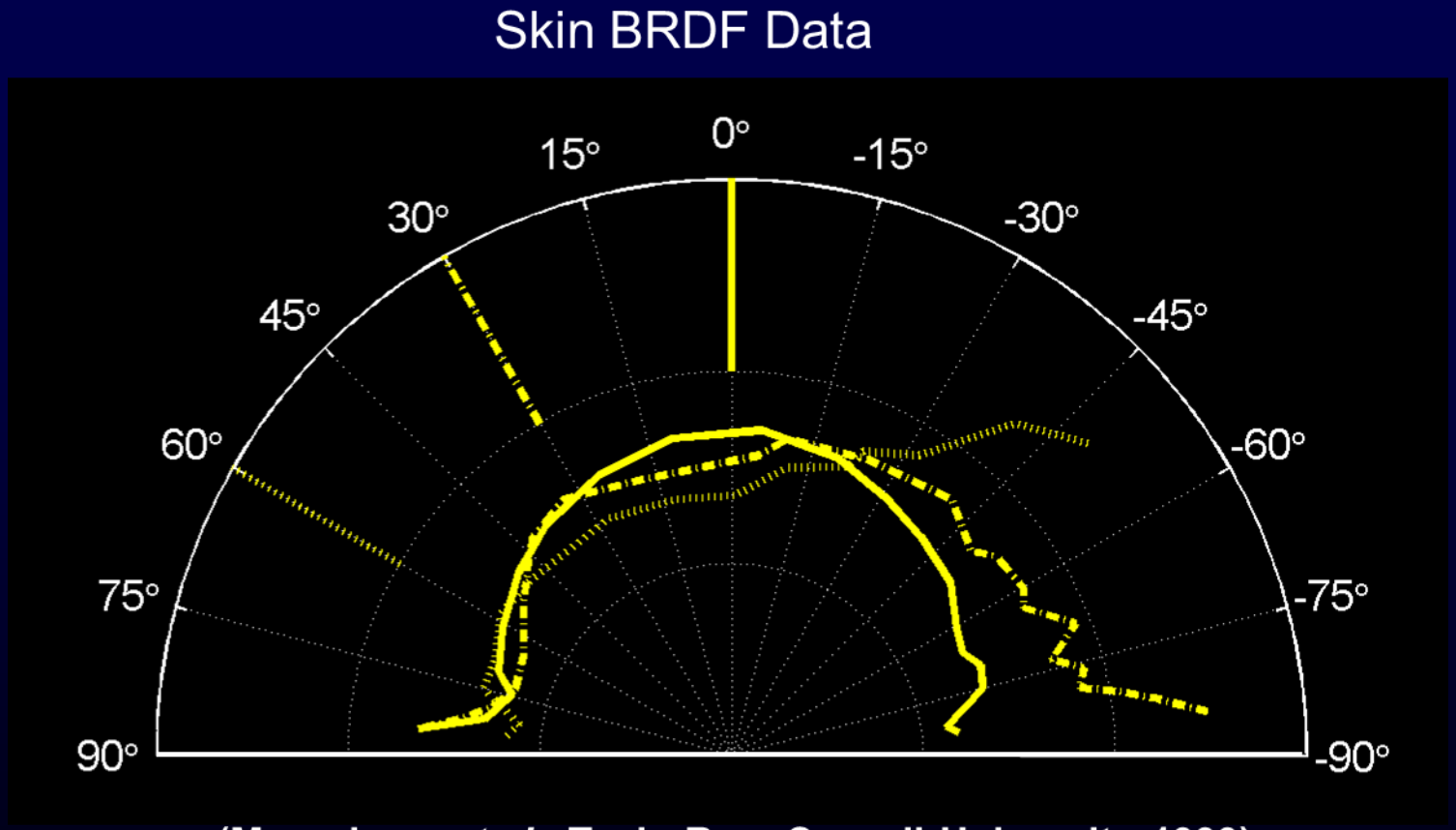


- Measurements are usually limited to a few incidence and collection geometries

Reflectance and Transmittance Measurement Geometries



- Scattering measurements are usually limited to a few representative cases



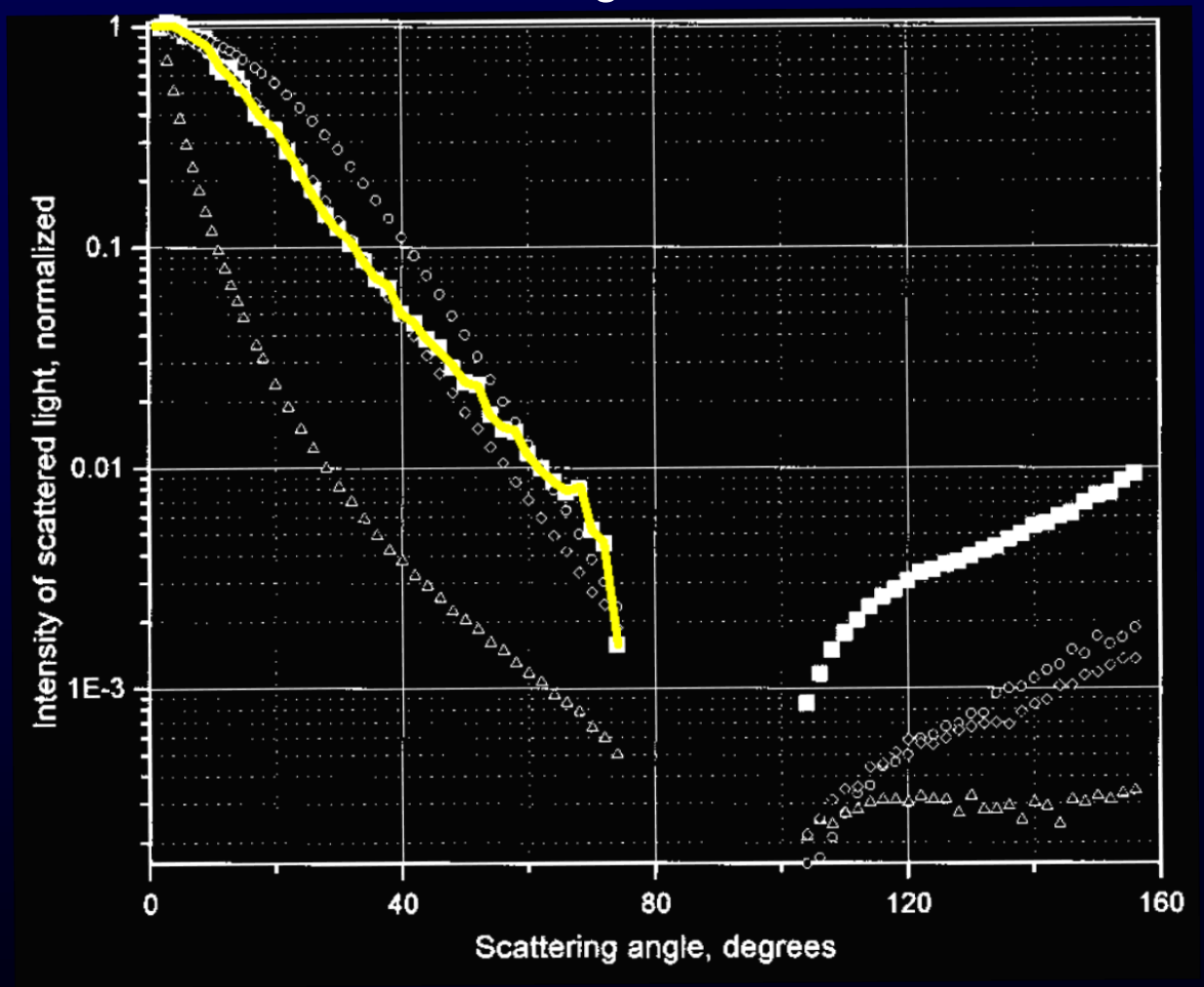
(Marschner *et al.*, Tech. Rep. Cornell University 1999)

- 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

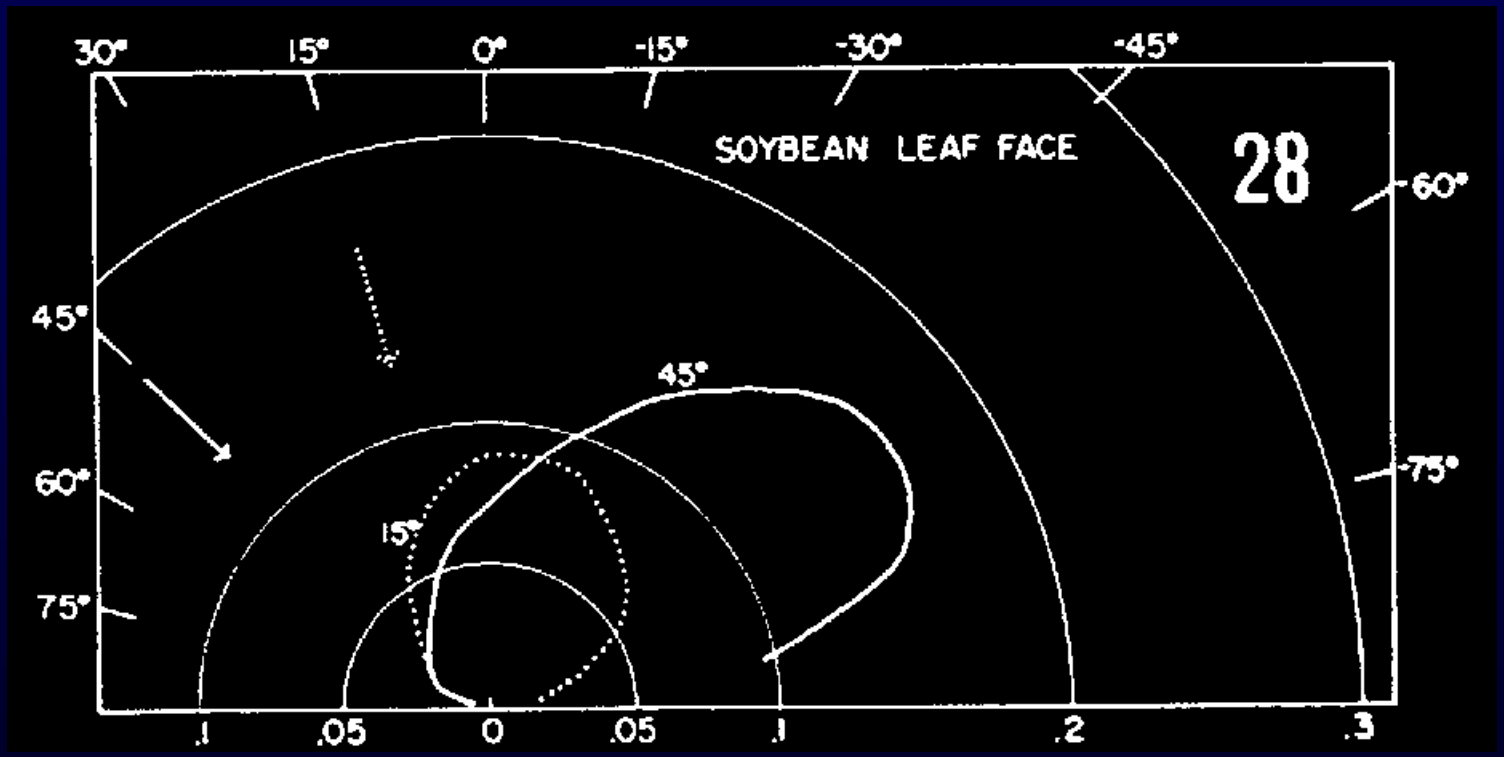
- Measured data is rarely available electronically

Blood Scattering Data at 613 nm



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

BRDF Data for a Soybean Leaf



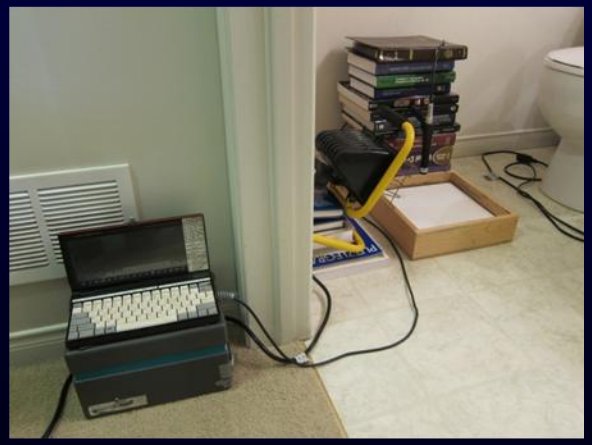
(Woolley, Plant Physiology 1971)

How can we extract this data?

Outline

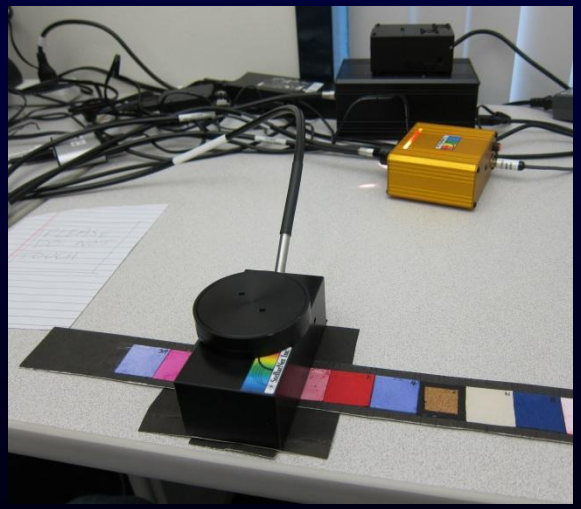
- ✓ What data?
- ✓ Biophysical Data Constraints
- ✓ Characterization Data Constraints
- ✓ Evaluation Data Constraints
- ❑ Getting Our Own Data

Getting Our Own Data



- Investments
  - Equipment
  - Space
  - Time

- Benefits
  - Control
  - Contributions

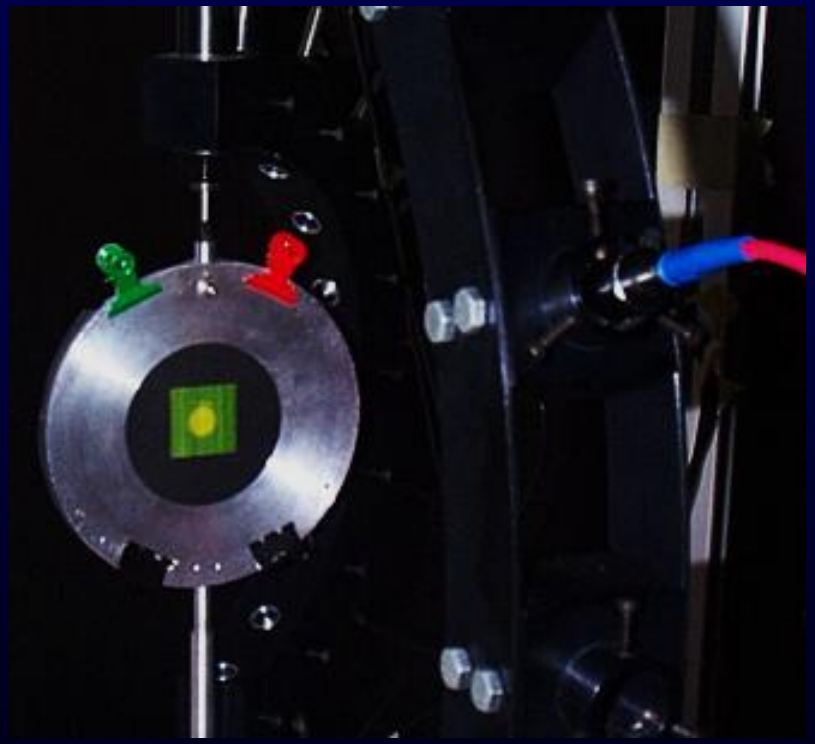


- Investments
  - Equipment
  - Space
  - Time
- Benefits
  - Control
  - Contributions

(Chen and Baranoski, Optics Express 2008)

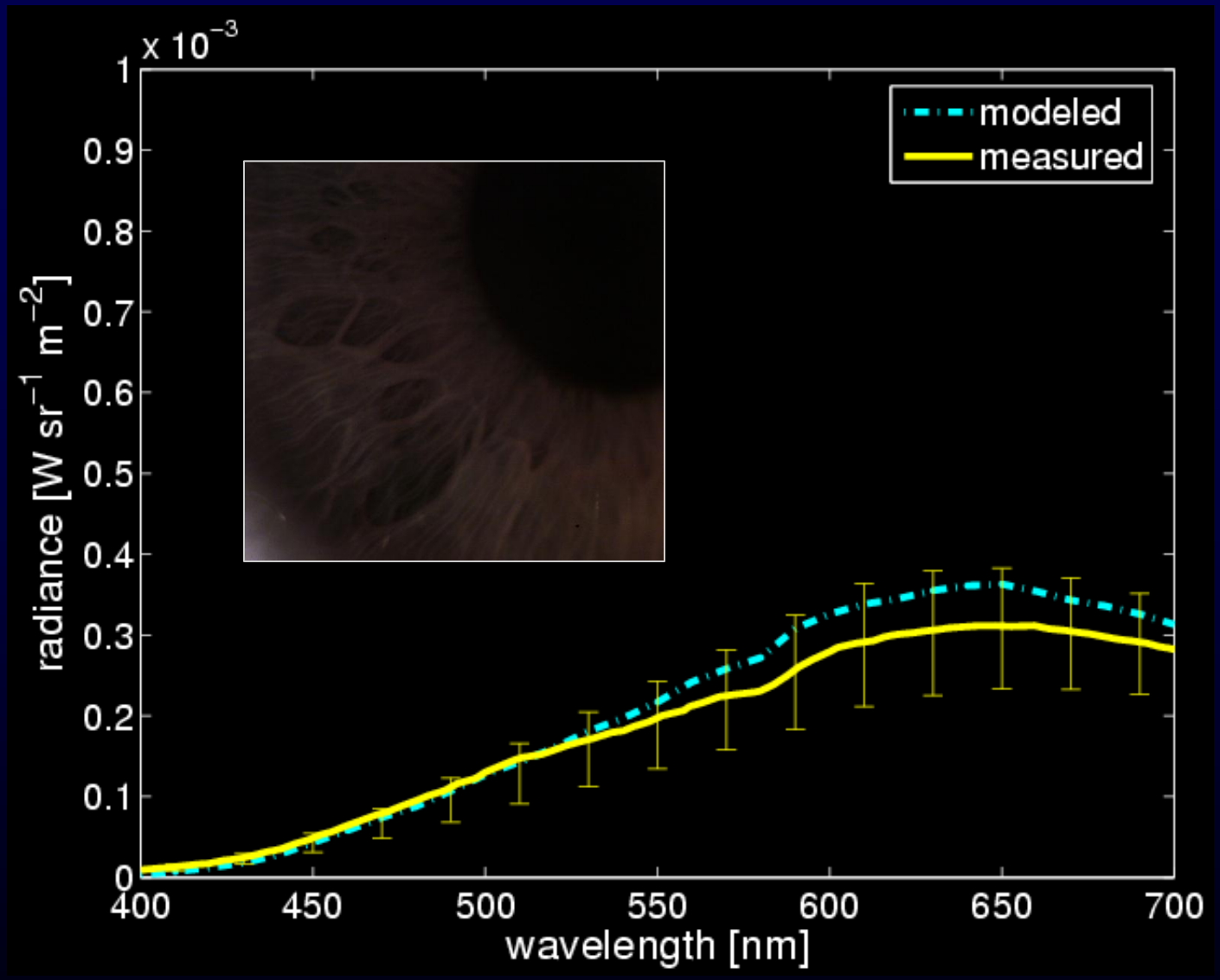
- Investments and benefits may increase considerably when it comes to scattering measurements

BTDF and BRDF Measurement Arrangements



- Investments and benefits can increase even more when comes to human data

Iridal Spectral Data



(Imai, Tech. Rep. RIT 2000)

Photorealistic Models for Pupil Light Reflex and Iridal Pattern Deformation

Vitor F. Pamplona
Manuel M. Oliveira
Gladimir V. G. Baranoski

- In our search for data, we cannot lose sight of something even more fundamental:

"The essence of science is
independent thinking and hard work,
not equipment."

C.V. Raman

This concludes Lecture 2!

Thanks!

Questions?

Credits: Images and Photos

- J. Rokne
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