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

Lecture Series

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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

# Model Design: Balancing Reality and Abstraction

*Lecture 3*

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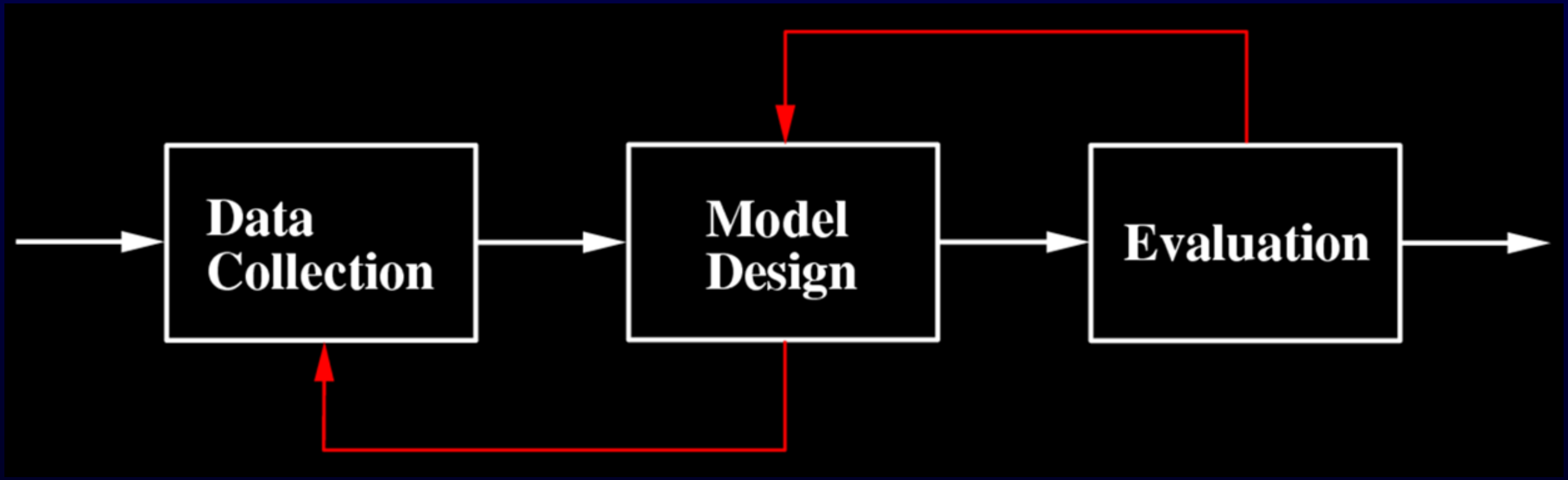
# Outline

- ❑ Drawing Board
- ❑ Simulation Approaches
- ❑ Level of Abstraction
- ❑ Design Evolution
- ❑ Iterative Refinement

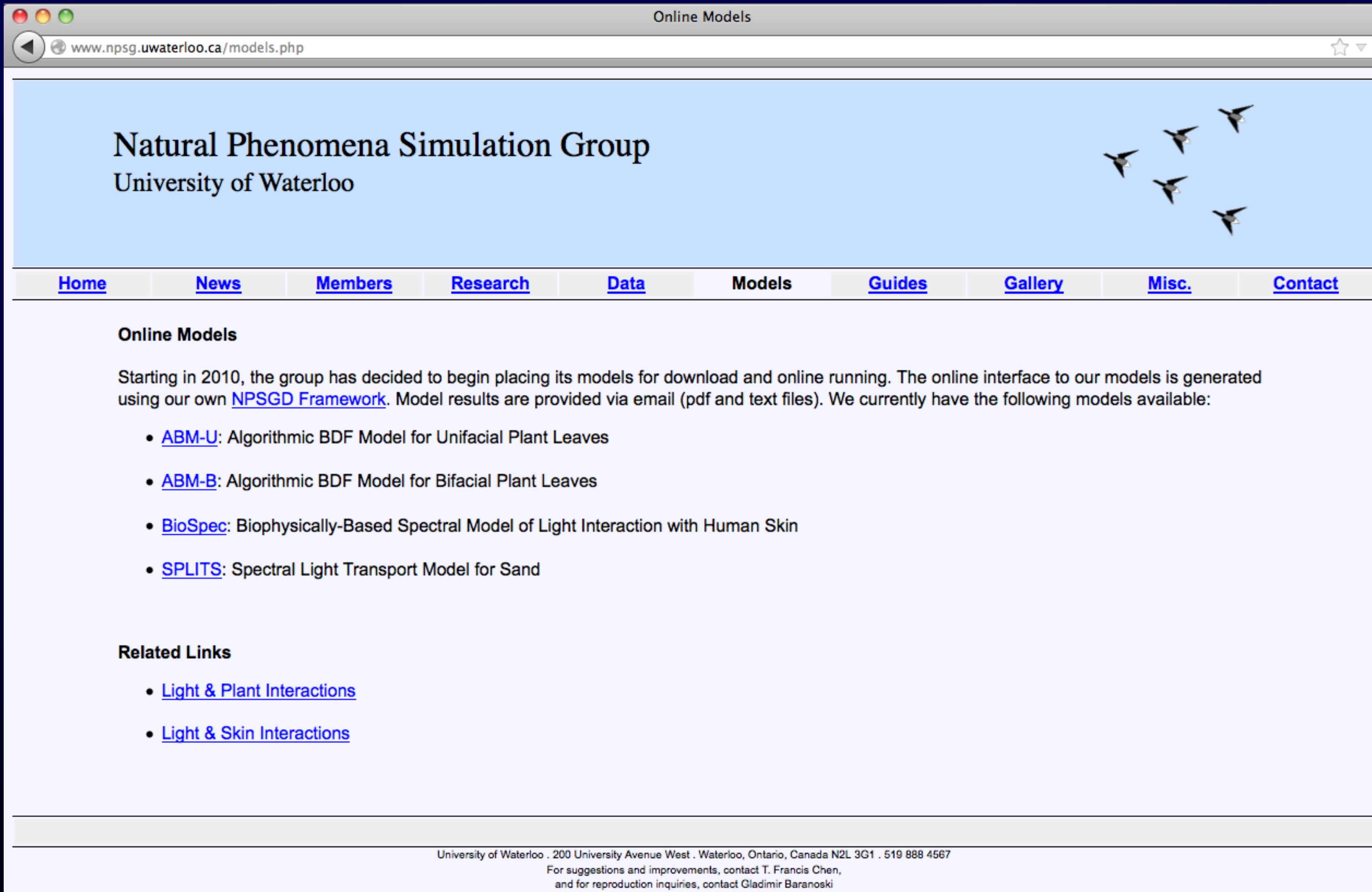
# Drawing Board

- Top-down vs. Bottom-up Design Strategies



- Light interaction models developed by the NPSG:
  - For plant leaves: ABM (Eurographics 1997), ABM-B and ABM-U (Remote Sensing of Environment 2006)
  - For human skin: BioSpec (Eurographics 2004)
  - For human iris: ILIT (Eurographics 2006)
  - For sand: SPLITS (Optics Express 2007)
  - For human blood: CLBlood (Eurographics 2012)

- Supporting materials (code and data) can be found at:



# Simulation Approaches

➢ Radiative Transfer Approaches

- Successive scattering technique
- Ambartsumian’s method
- Discrete ordinate method
- Chandrasekhar’s X and Y functions
- Adding-doubling method

# Simulation Approaches

➢ Radiative Transfer Approaches

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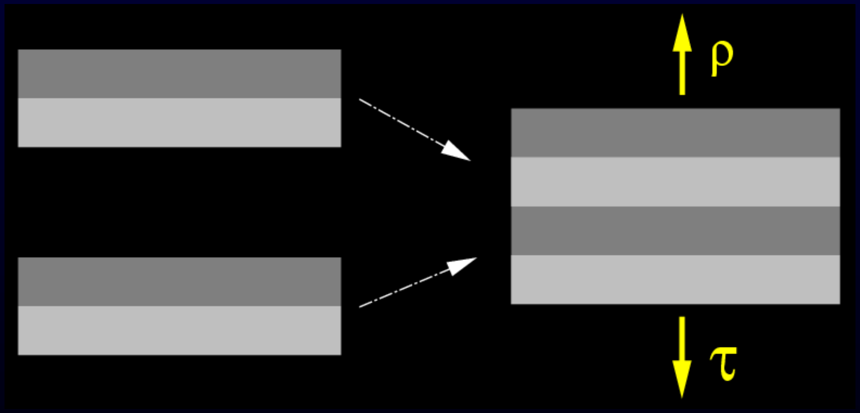
- Adding-doubling method

  - Adding method: uses the known reflectance and transmittance of two slabs to compute the reflectance and transmittance of another thin slab

  - Doubling method: computes the reflectance and transmittance of the target slab by doubling the thickness of the thin slab until it matches the thickness of the target slab



- Allow the rapid determination of optical properties through inversion procedures

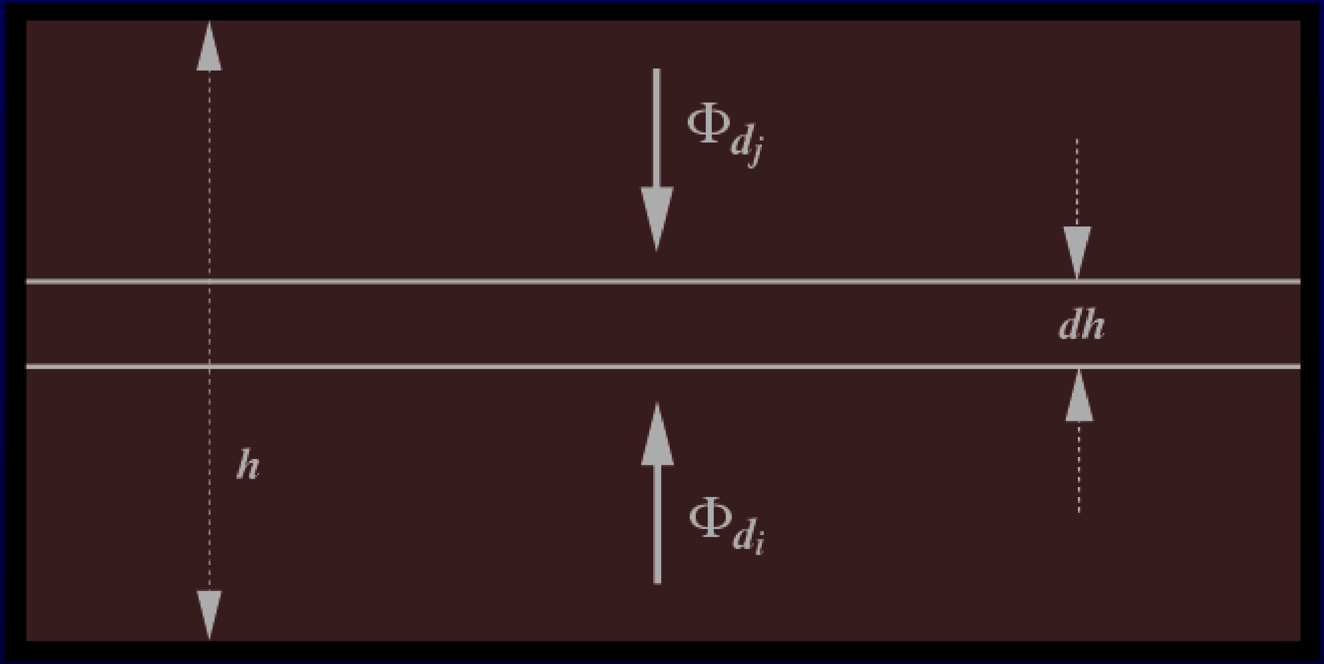
- Accuracy depends on the criteria applied to define a "sufficiently thin slab"

- Restrictions on the sample:

  - ❖ it must be uniformly illuminated
  - ❖ it must be homogeneous

## ➢ Kubelka-Munk Theory Based Approaches

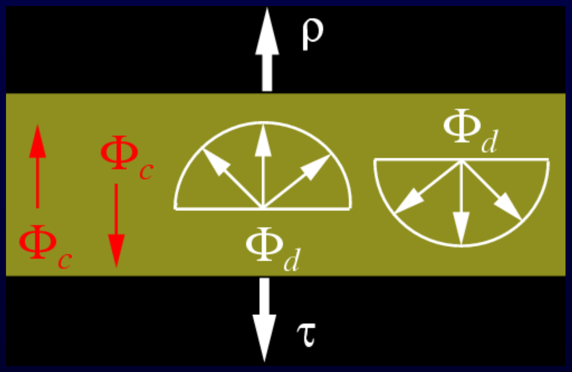
- Kubelka-Munk (K-M) theory (1931)
  - It applies energy transport equations to describe the radiation transfer in diffuse scattering media
  - Parameters: scattering and absorption coefficients
  - Two fluxes: diffuse downward and upward
  - The relations between the fluxes are expressed by linear differential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




$$-d\Phi_{d_j} = -(\mu_a + \mu_s)\Phi_{d_j} dh + \mu_s \Phi_{d_i} dh$$

$$d\Phi_{d_i} = -(\mu_a + \mu_s)\Phi_{d_i} dh + \mu_s \Phi_{d_j} dh$$

- K-M (flux) approaches used in tissue 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




  - Accuracy and sample restriction issues
  - Allow the rapid determination of optical properties (*e.g.*, absorption and scattering coefficients) through inversion procedures

## ➢ Diffusion Theory Based Approaches

- Boltzmann photon transport equation
  - It can an be used to describe photon propagation in optically turbid media
  - Requires the optical properties of the medium to be expressed in terms of scattering coefficient, absorption coefficient and phase function

- Diffusion theory

  - Approximate solution of the Boltzmann equation

  - Assumes a scattering-dominated light transport

  - Combines the scattering coefficient and the phase function asymmetry factor in one parameter:

reduced scattering coefficient

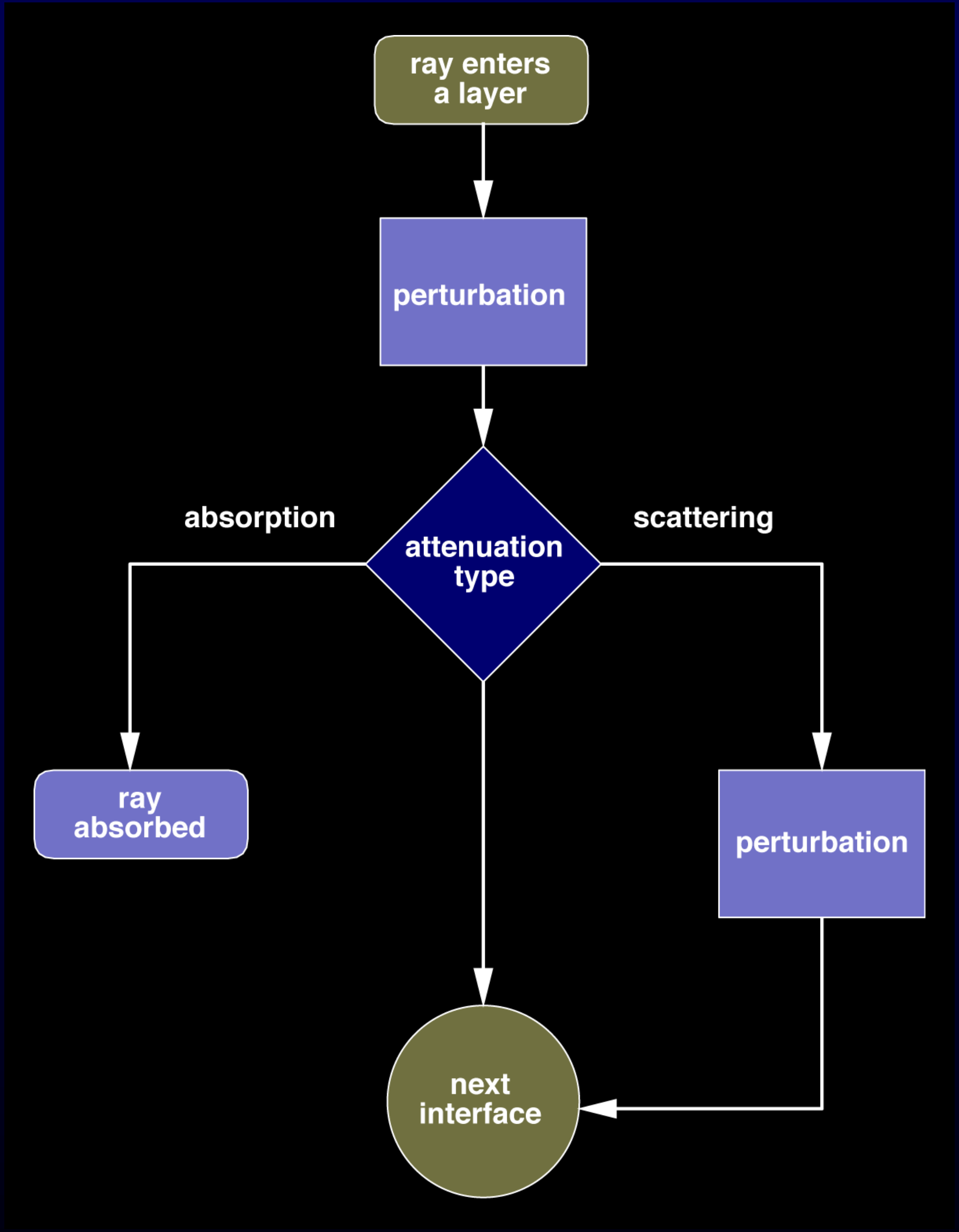
$$\mu_s{}' = \mu_s(1-g)$$

- Approaches based on the diffusion theory:
  - are amenable to analytic manipulation
  - place minor constraints on the type of sample
  - are relative easy to use
  - provide a **poor** approximation when the absorption coefficient of a turbid medium is **not** significantl smaller than the scattering coefficient

# ➢ Monte Carlo Based Approaches

- Monte Carlo method
  - Originally proposed by Metropolis and Ulam (1949) to stochastically simulated radiative transfer processes
  - Idea: to keep track of photon histories as they are scattered and absorbed within the material
  - Extensively employed in many fields, from biomedical optics to remote sensing

Example:



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


- Pros and cons:
  - Relatively easy to implement (algorithmic formulation)
  - Sufficiently flexible to allow the simulation of complex materials
  - Accuracy of the simulations is bounded by the accuracy of the input parameters and the proper representations of the mechanisms of scattering and absorption
  - Computationally intensive

# Outline

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# 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!"

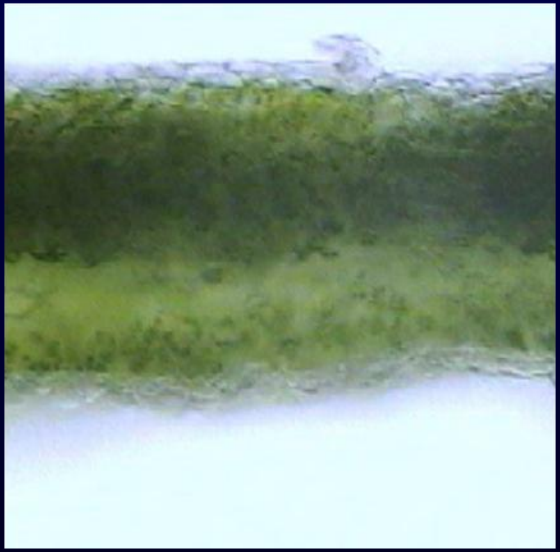
M.G.J. Minnaert (1974)
*Light and Color in the Outdoors*

## ➢ How can we represent real materials?

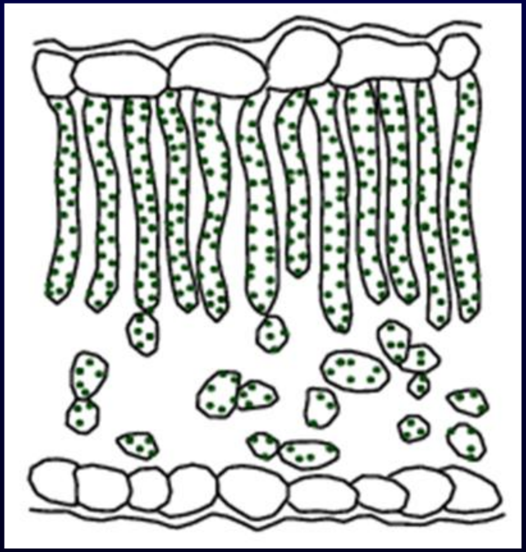
- Example: plant leaves

Bifacial Leaves

Cross-Section (OM)

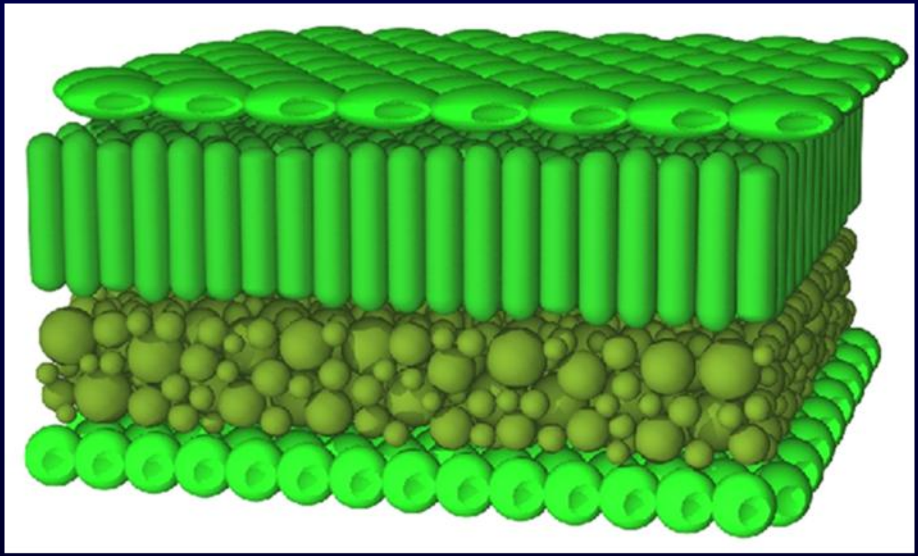


Cross-Section (sketch)



- How about considering the full material description?

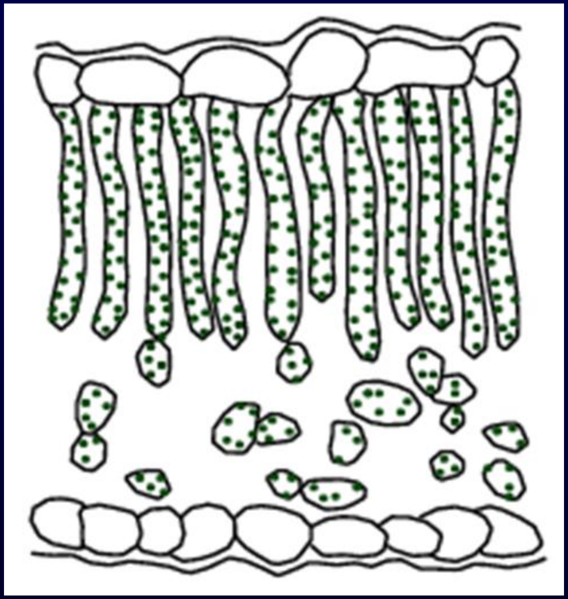
3D Representation Used by the Raytran Model



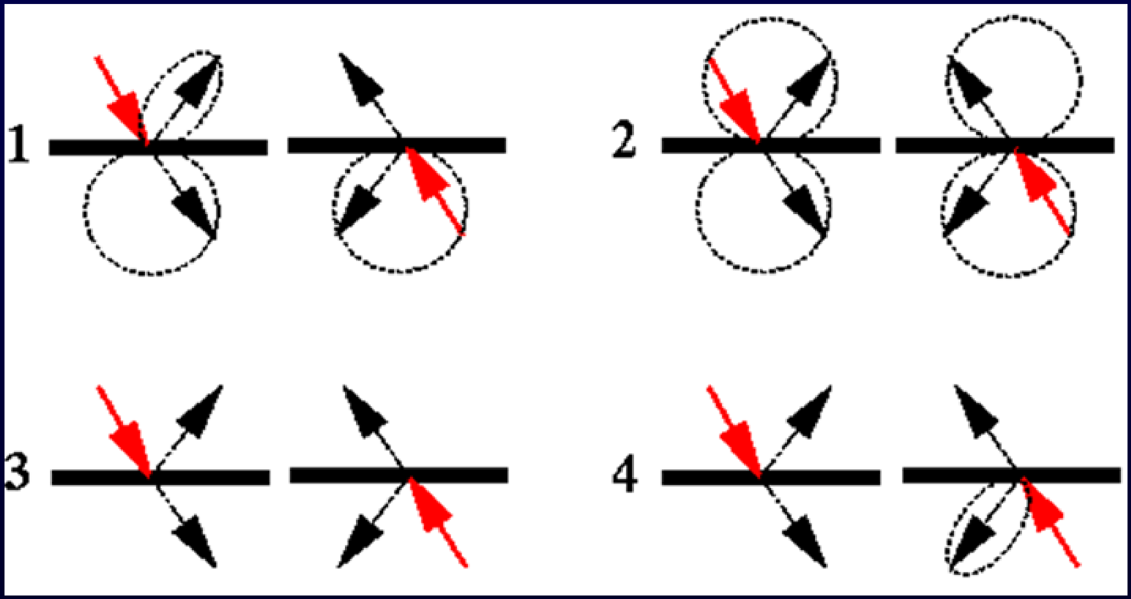
(Govaerts *et al.*, Applied Optics 1996)

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

Cross-Section

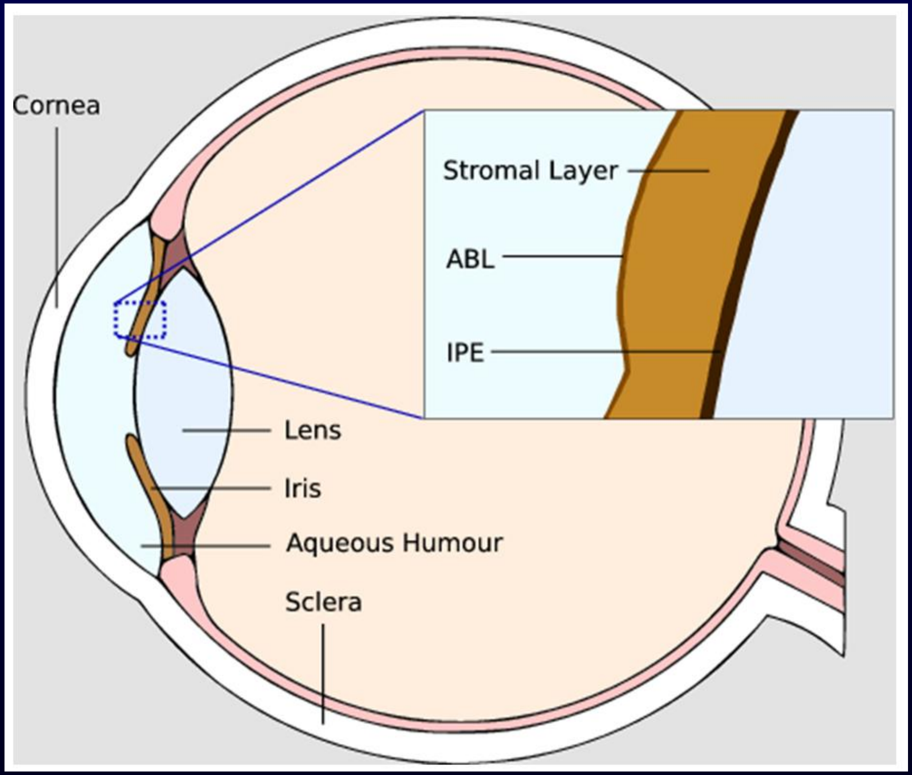


Layered ABM Model for Plant Leaves

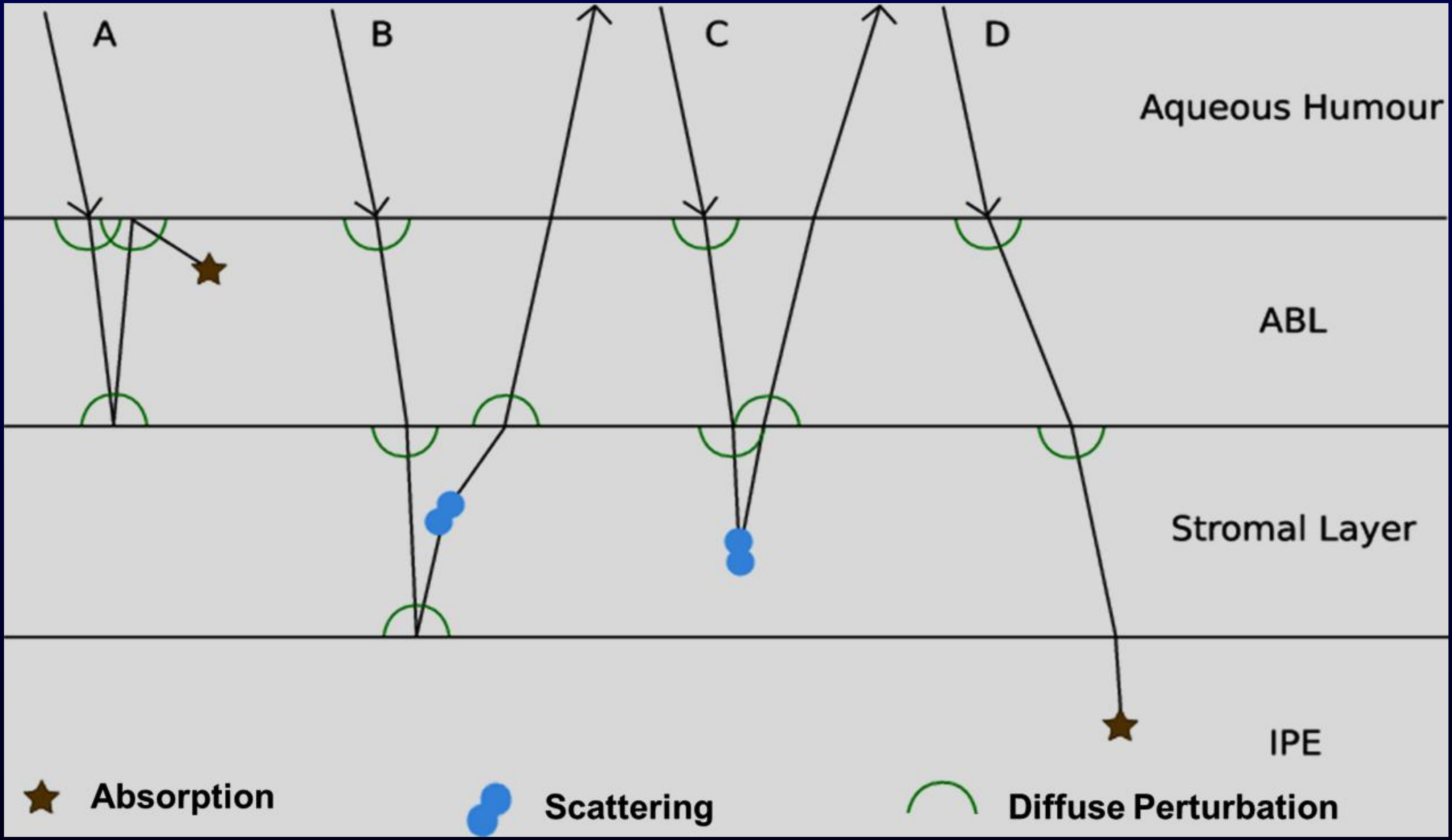


Human Eye

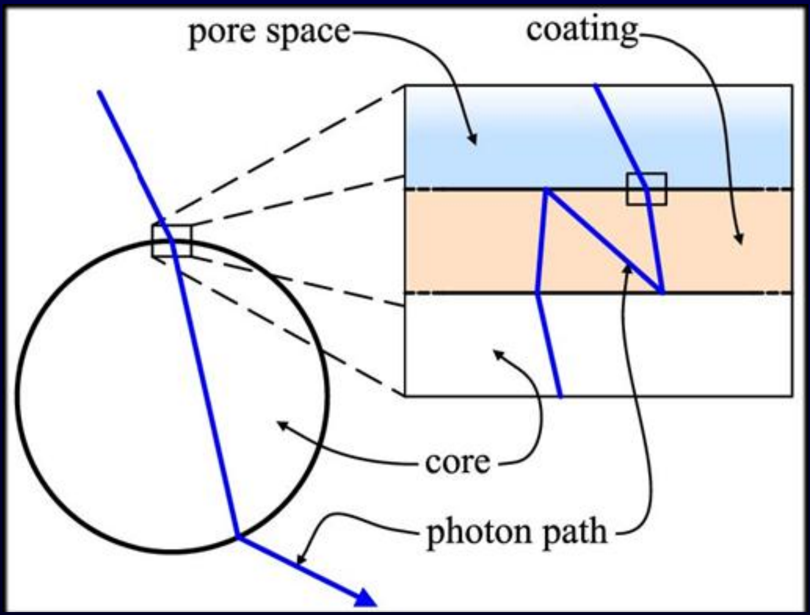
Cross-Section of Ocular Tissues



# Examples of Ray (light) Propagation/Attenuation Processes Taken into Account by the Layered ILIT Model

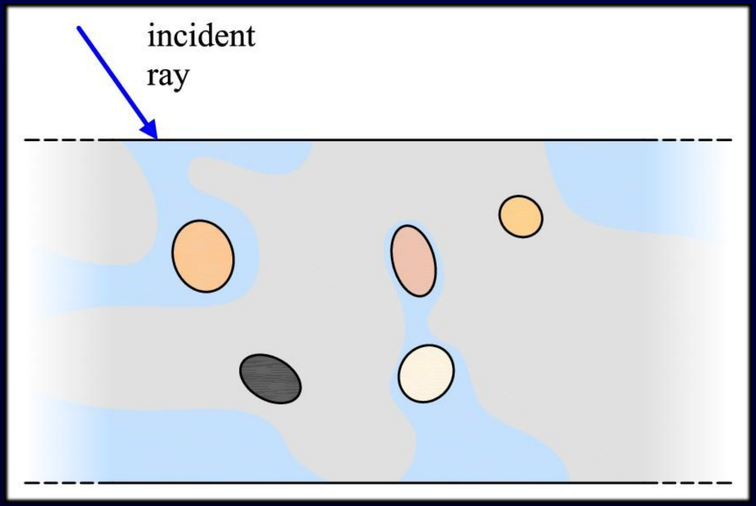


- How about combining both approaches?
  - SPLITS model considers the light interactions with individual sand grains and within each layer of a sand grain coating

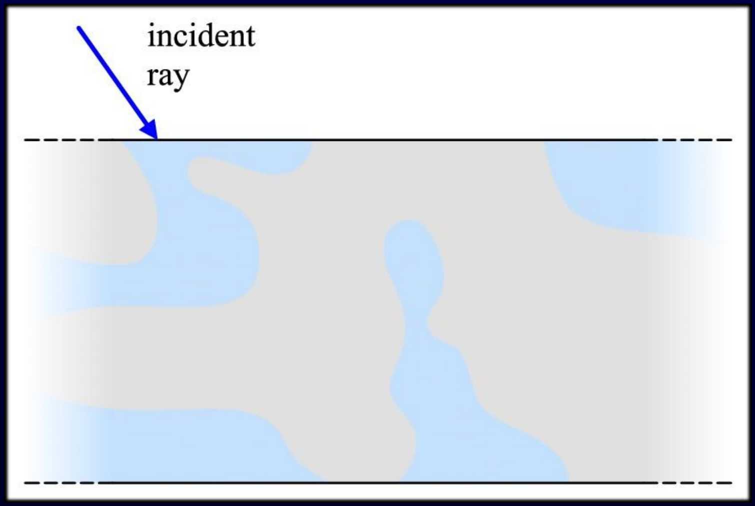



  - SPLITS generates sand grains on the fly during the simulations

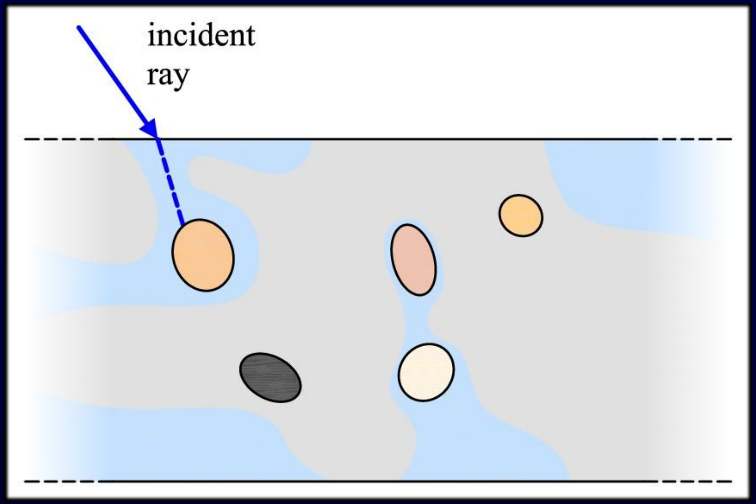
Ray Tracing



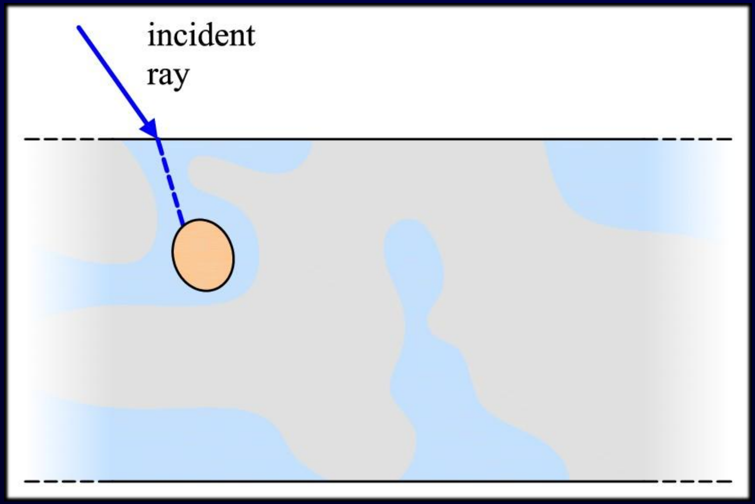

SPLITS



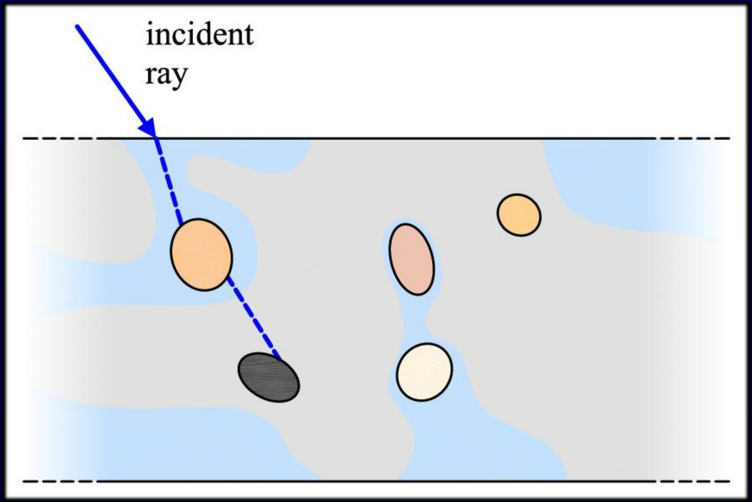
Ray Tracing



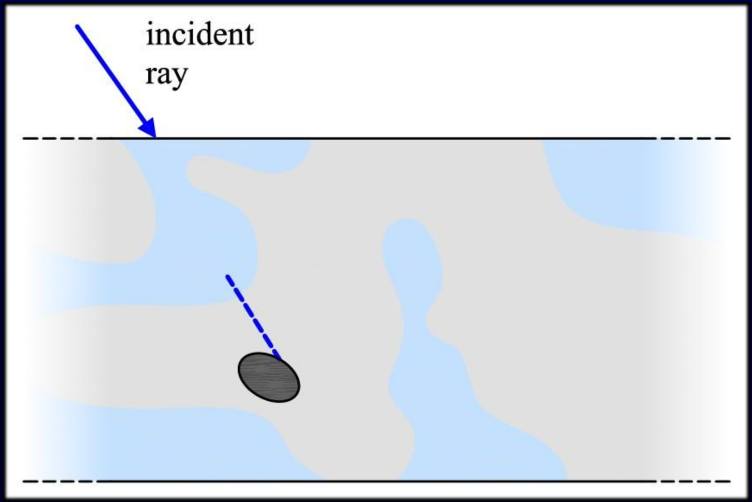

SPLITS



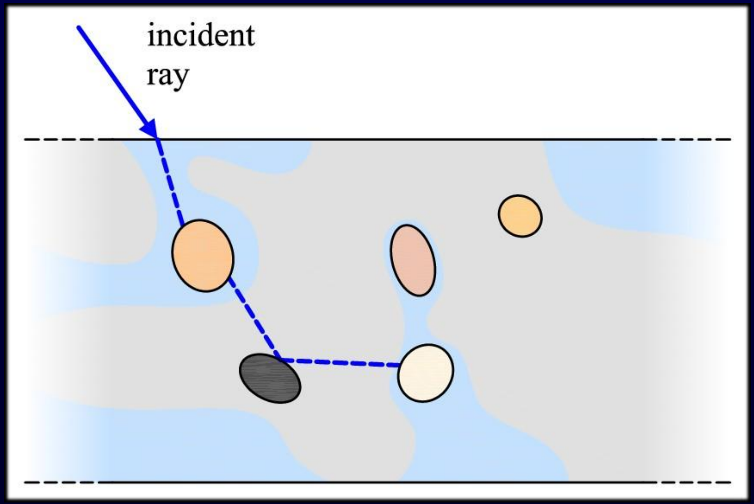
Ray Tracing



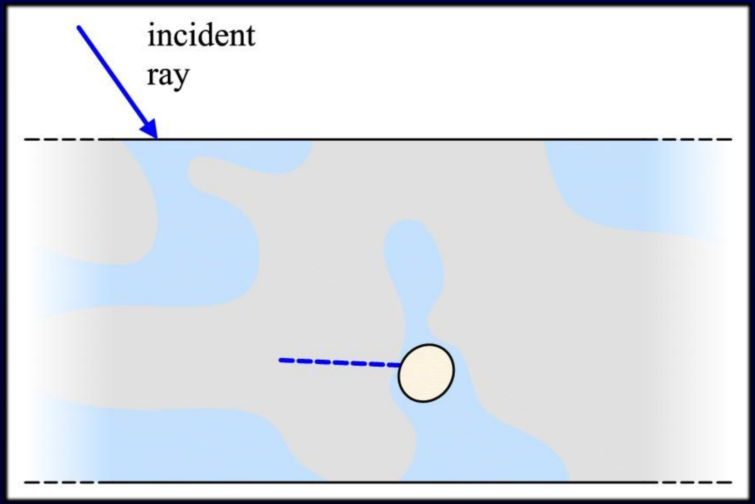

SPLITS



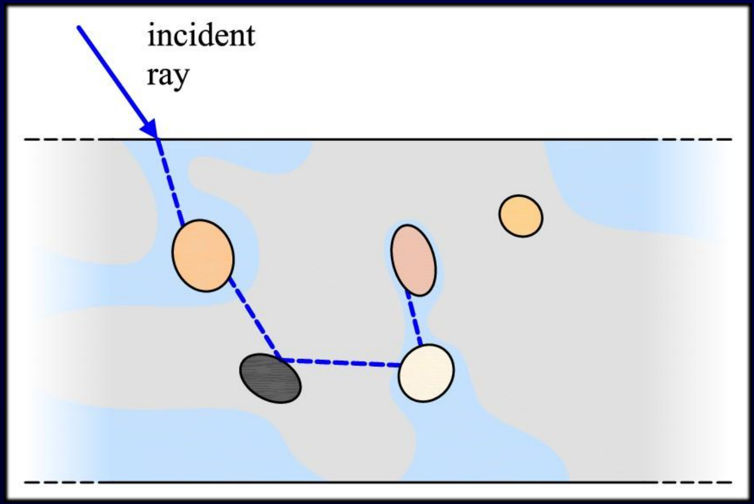
## Ray Tracing



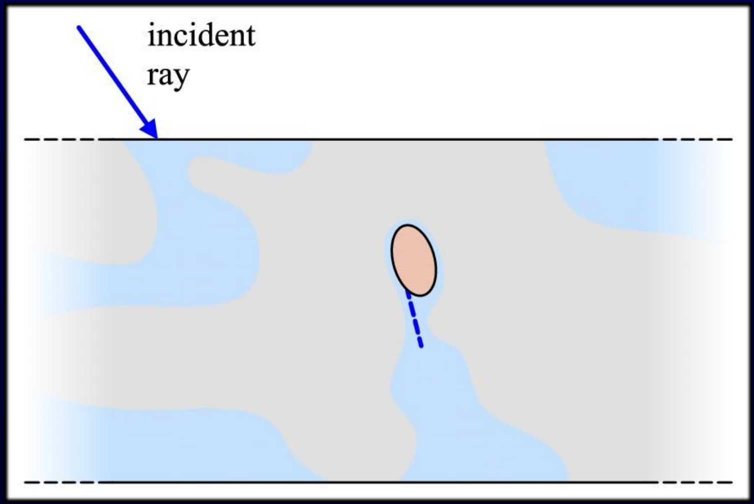

## SPLITS



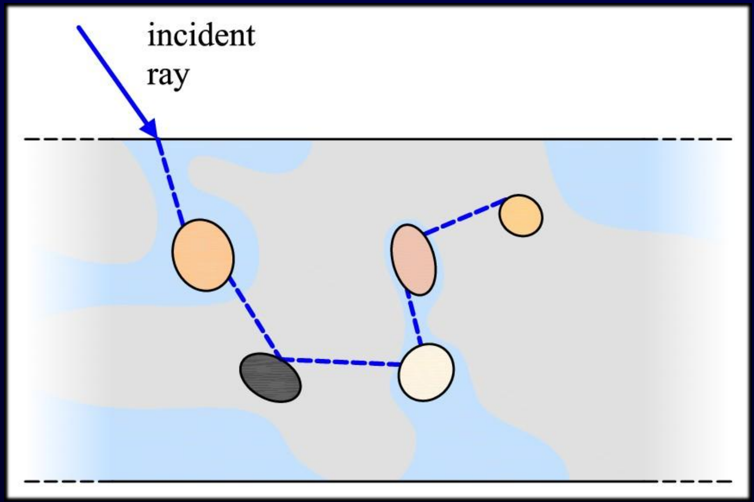
Ray Tracing



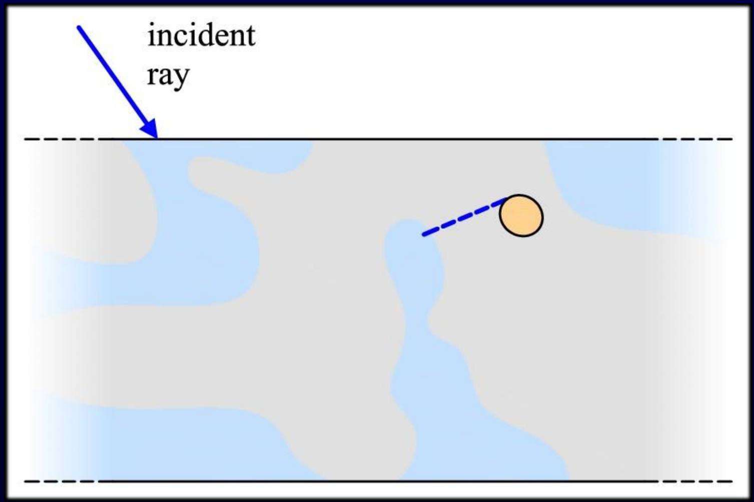

SPLITS



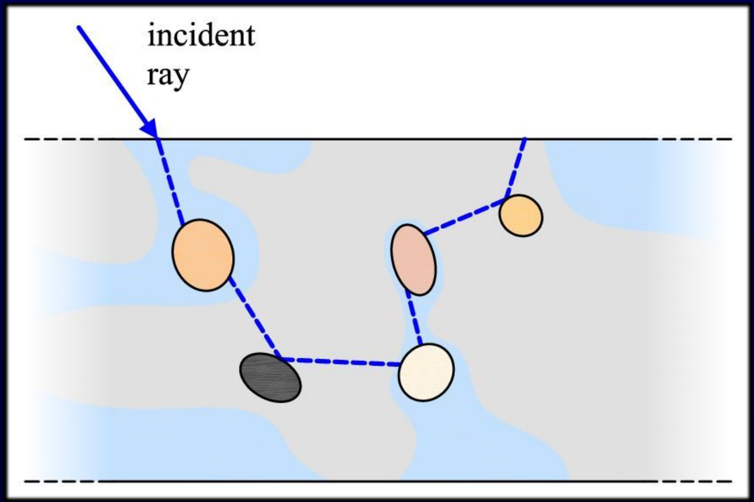
Ray Tracing



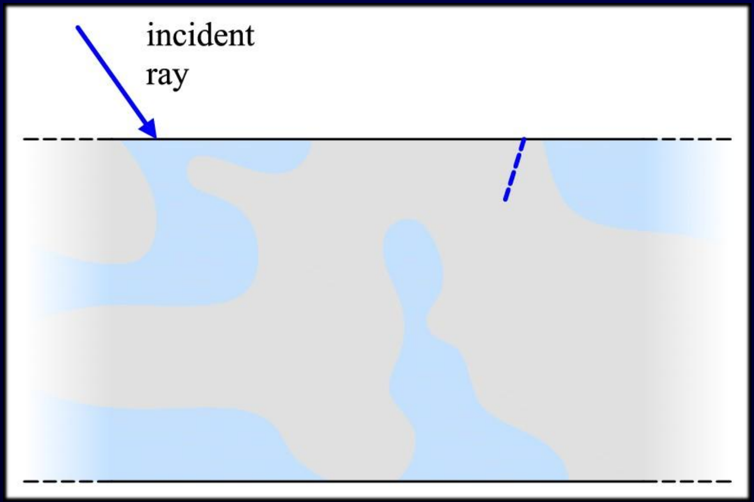

SPLITS



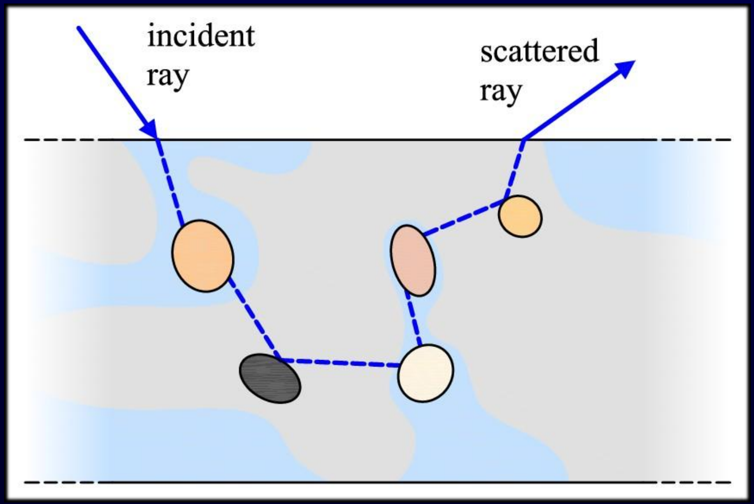
Ray Tracing



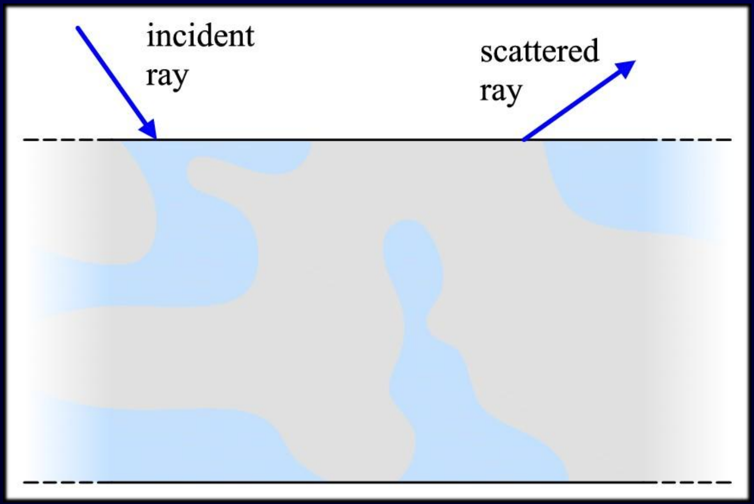

SPLITS



## Ray Tracing



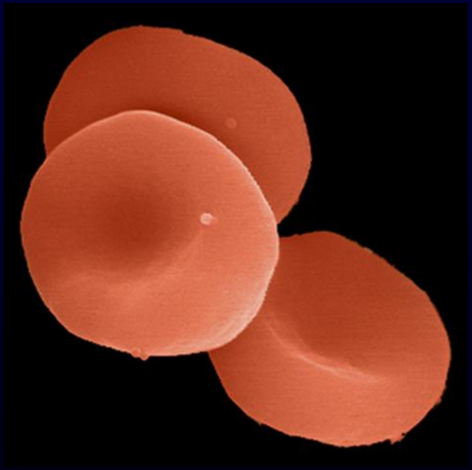

## SPLITS



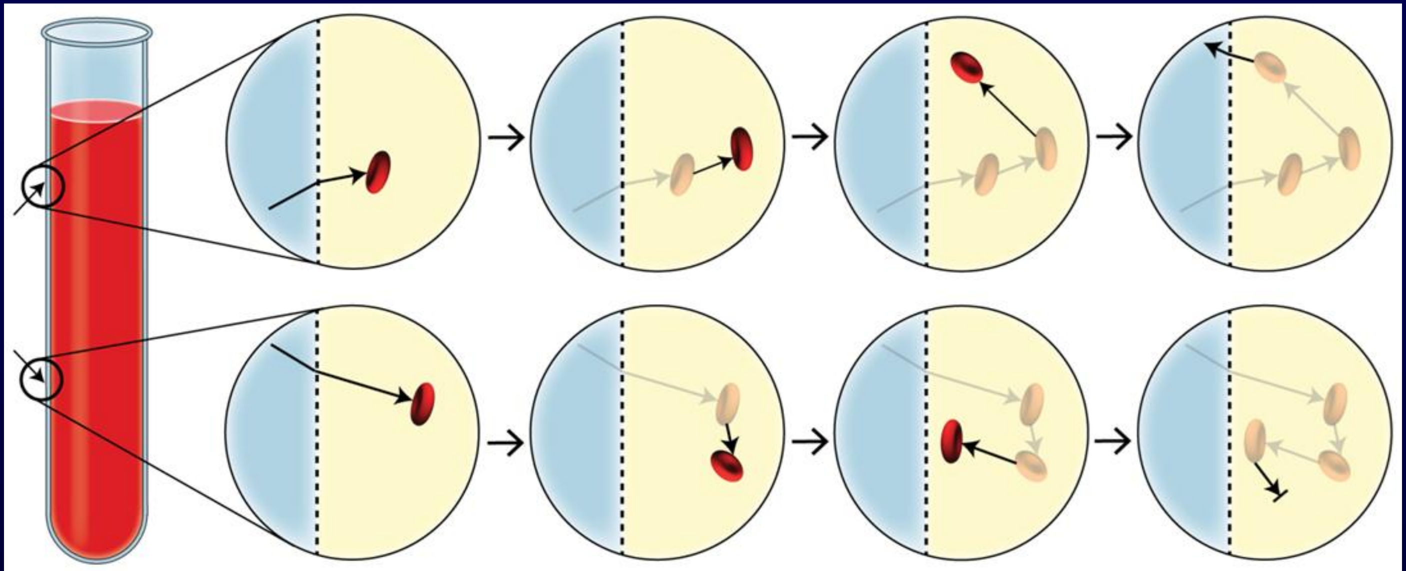
- Recently, the “SPLITS approach” was employed in the the development of a new cell-based model of light interaction with human blood (CLBlood)

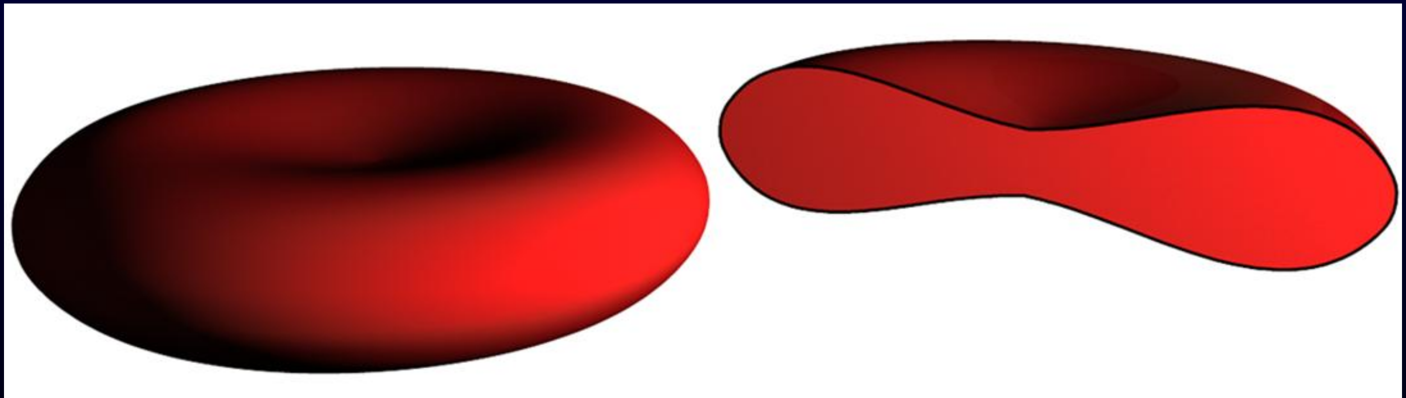
- Blood is composed of formed elements (mostly red blood cells, ~99%) suspended in a fluid called plasma

- Hematocrit (HCT) is the clinical term to describe percent of the blood volume occupied by red blood cells (RBCs)



Examples of ray (light) propagation/attenuation processes taken into account by the CLBlood model



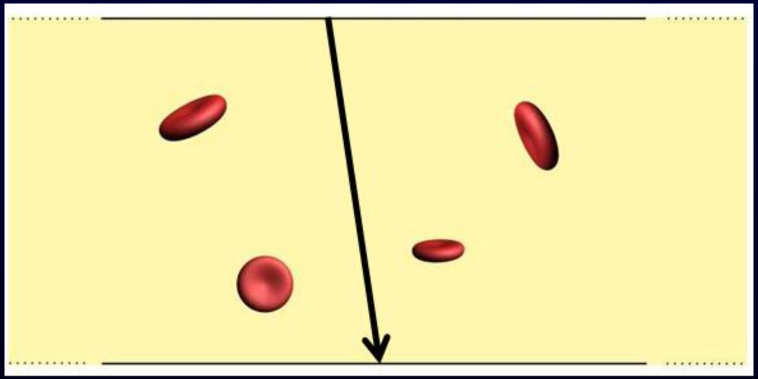


- In summary:
  - There are different ways to represent the materials
  - No approach is superior in all cases
  - The best approach for a given application will depend on:
    - data constraints
    - accuracy requirements
    - performance requirements
    - usability requirements

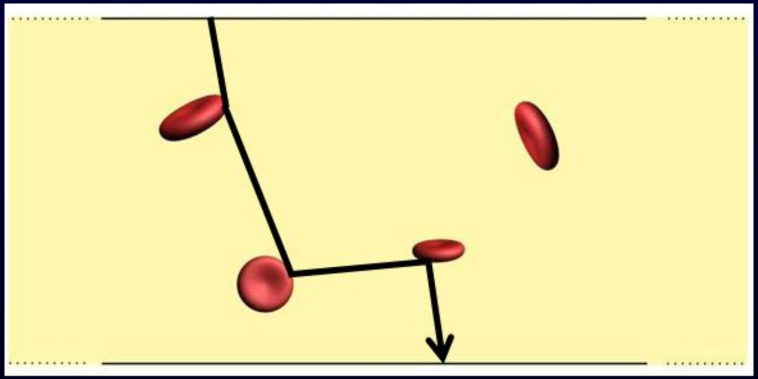
## ➢ Be careful with simplifying assumptions

- Material is homogeneous
  - Example: optical behaviour of whole blood differs from that of a homogeneous solution with the same concentration of hemoglobin due to sieve and detour effects

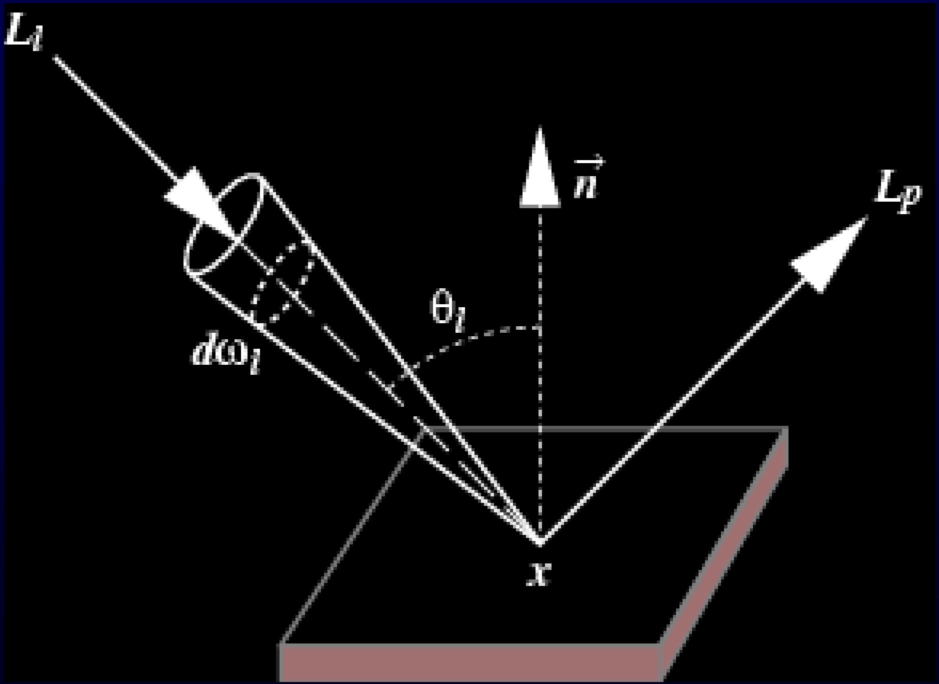
Sieve Effect



Detour Effect



- Material is isotropic



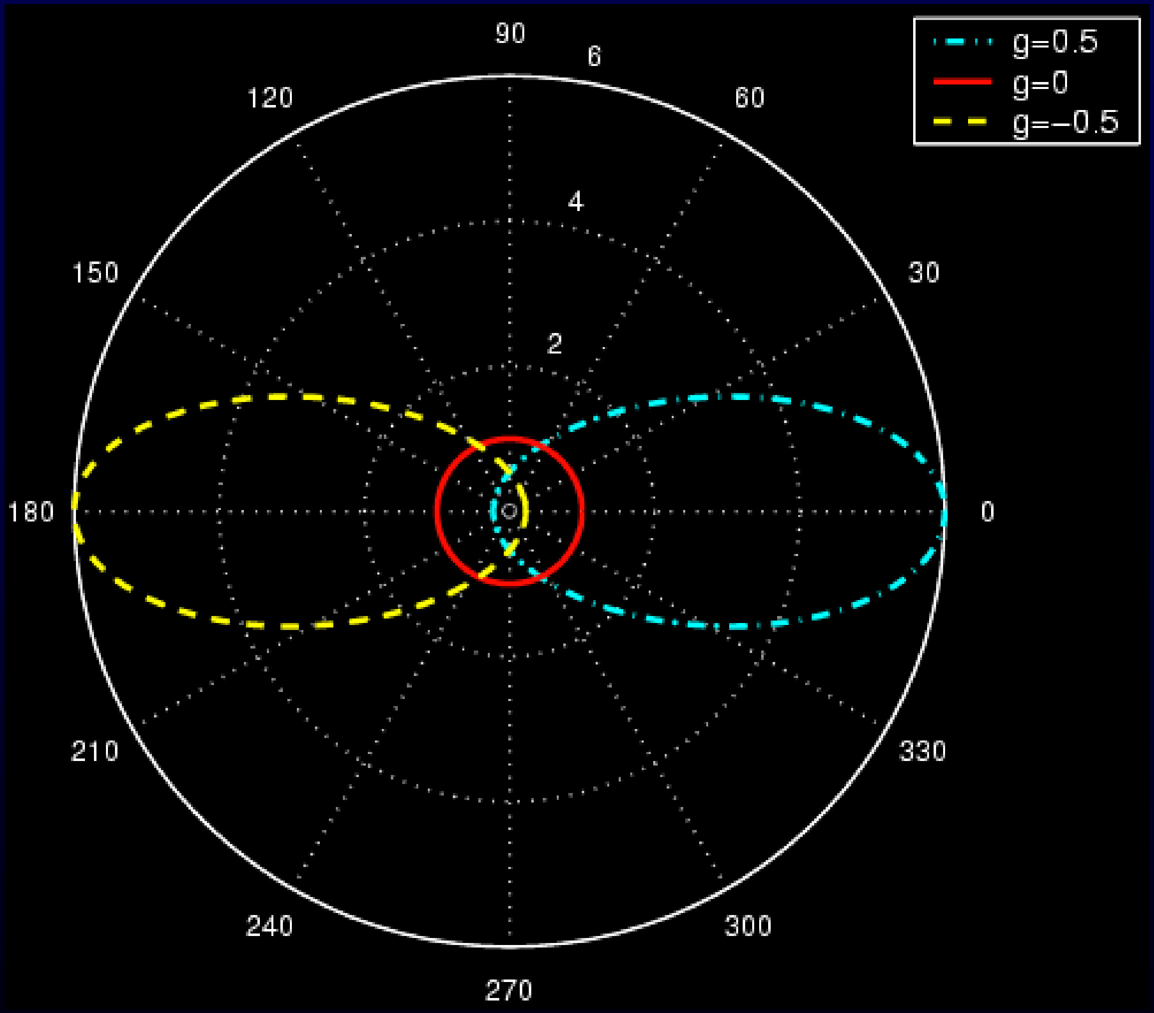
- Counter-example: plant leaves with parallel and reticular venation systems

## ➢ Be aware of unsound generalizations

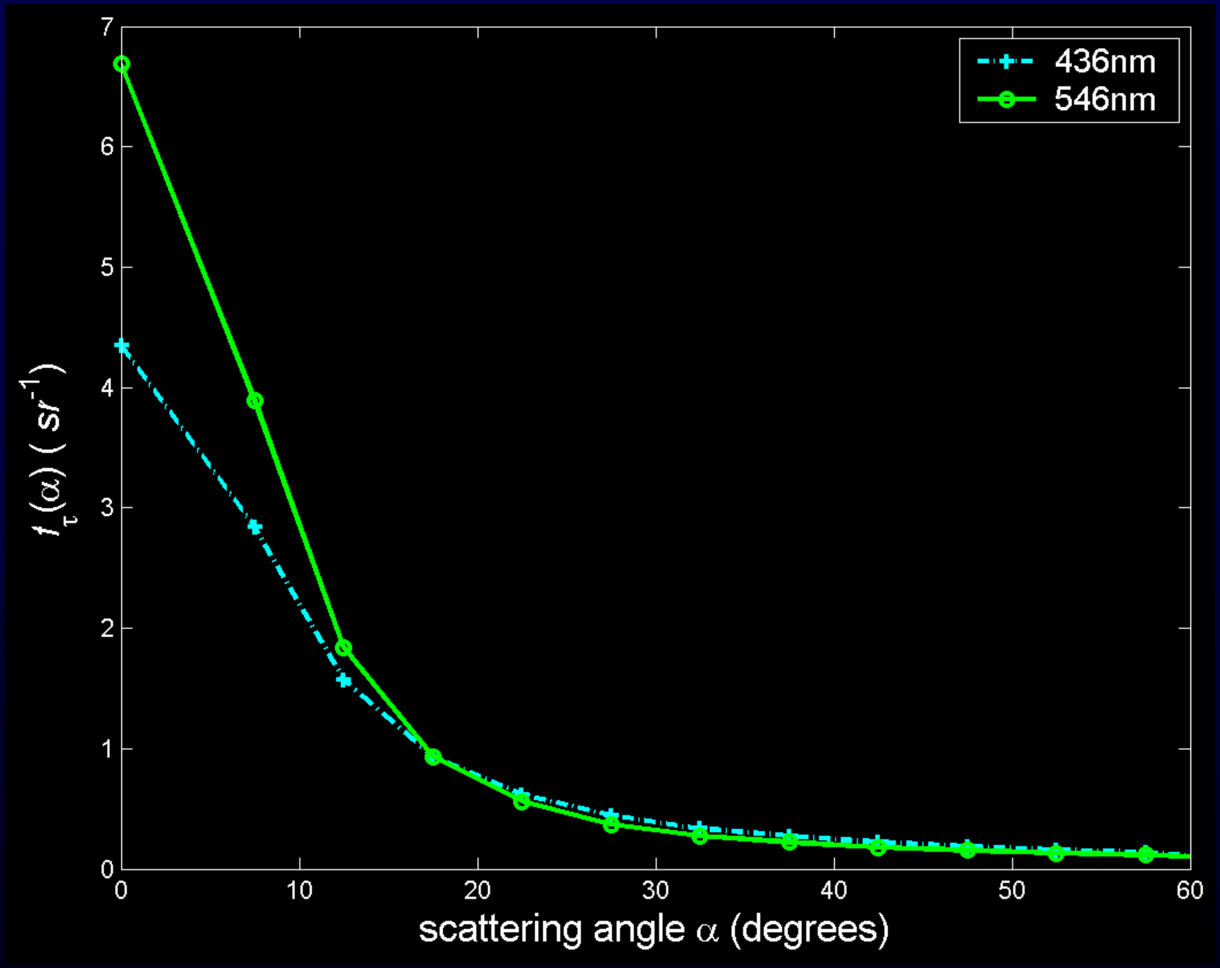
- Use of phase functions to approximate bulk scattering:
  - Bruls and van der Leun (1984) suggested that the their measured skin subsurface scattering data (254nm, 302nm, 365nm, 436nm and 546nm) could be approximated by a phase function tabulated by van de Hulst …

… 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



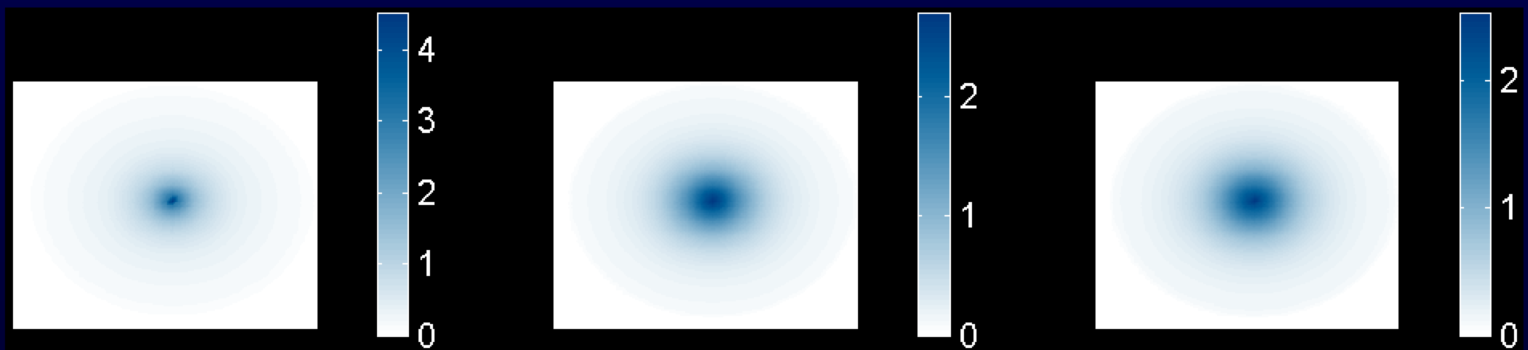
- Jacques *et al.* (1987) tried to approximate the measured scattering profile (laser) of skin dermis using the HGPF

- Yoon *et al.* (1987) used a similar approach for human aorta (laser)

- van Gemert *et al.* (1989) attempted to fit the HGPF (using least squares method) to the data measured by Bruls and van der Leun and dermis data (laser)

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

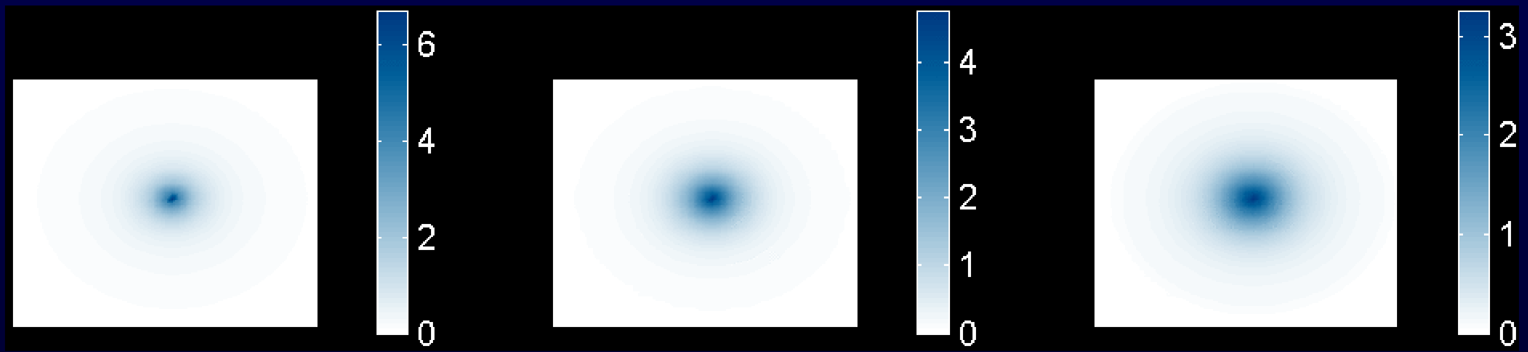
Measured | HGPF, *g*=0.761 | HGPF, *g*=0.748




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

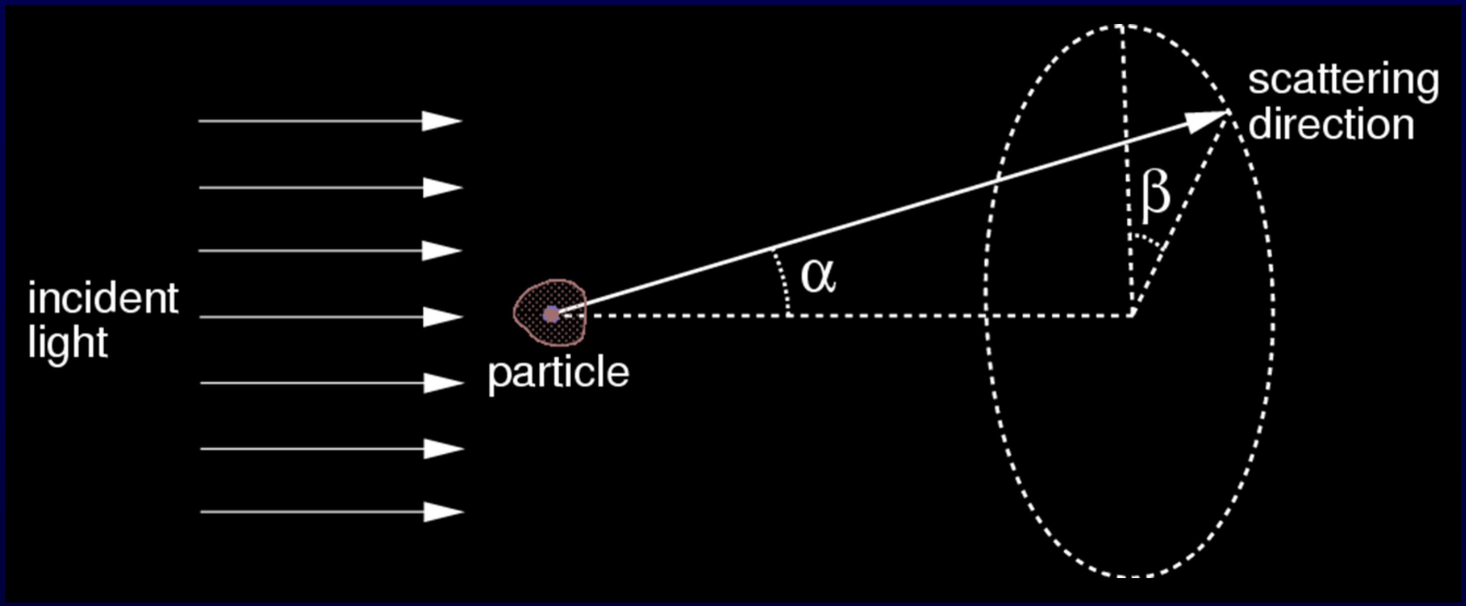
- Prahl's Monte Carlo based model (1988)

  - ❖ 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:

$\xi_1$ and $\xi_2$ = 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:

$\xi_1$ and $\xi_2$ = uniformly distributed random numbers $\in [0,1]$.

- Pros and cons of applying the HGPF in the simulation of light interaction with biological tissue:
  - 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 biological basis
  - it provides an accuracy/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

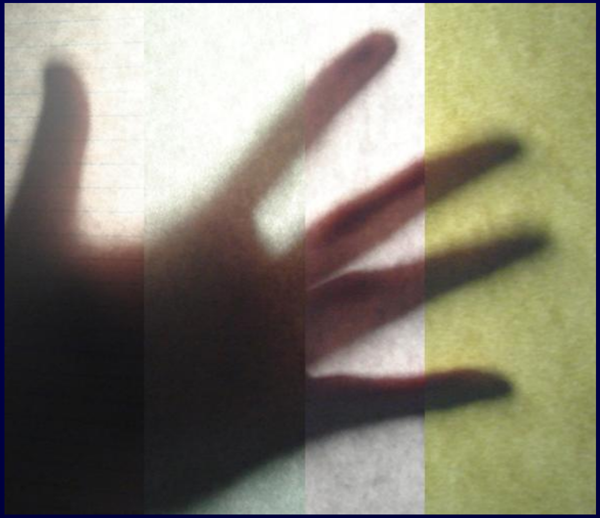
- Example: warping function derived from an exponentiated (*n*) cosine (EC) distribution

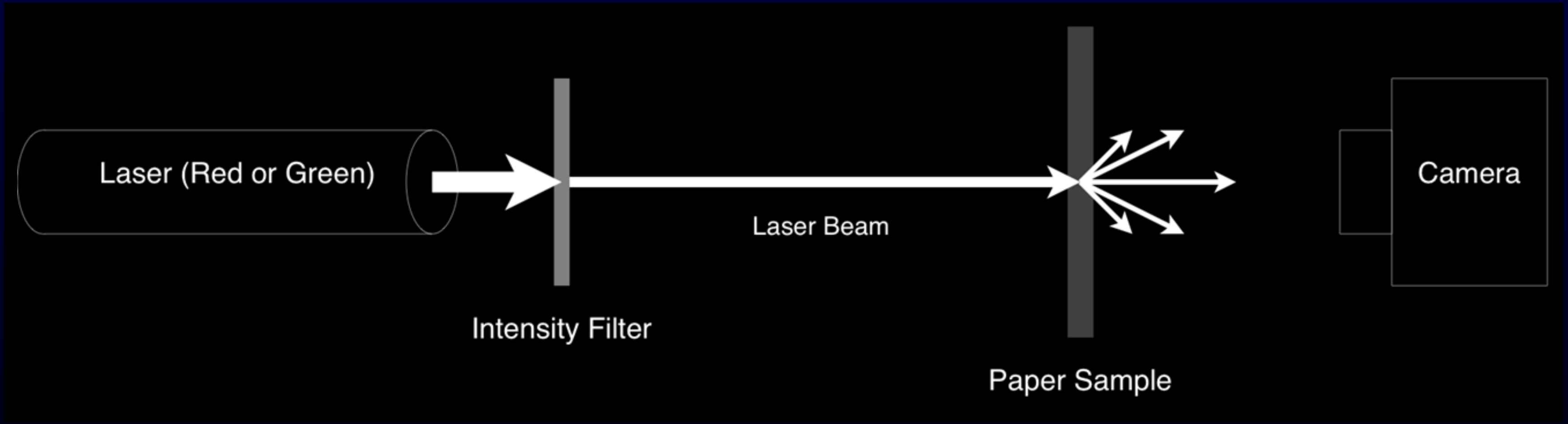
$$(\alpha, \beta) = (arccos(1-\xi_1)^{\frac{1}{n+1}}, 2\pi\xi_2)$$

where:

$\xi_1$ and $\xi_2$ = uniformly distributed random numbers $\in [0, 1]$.

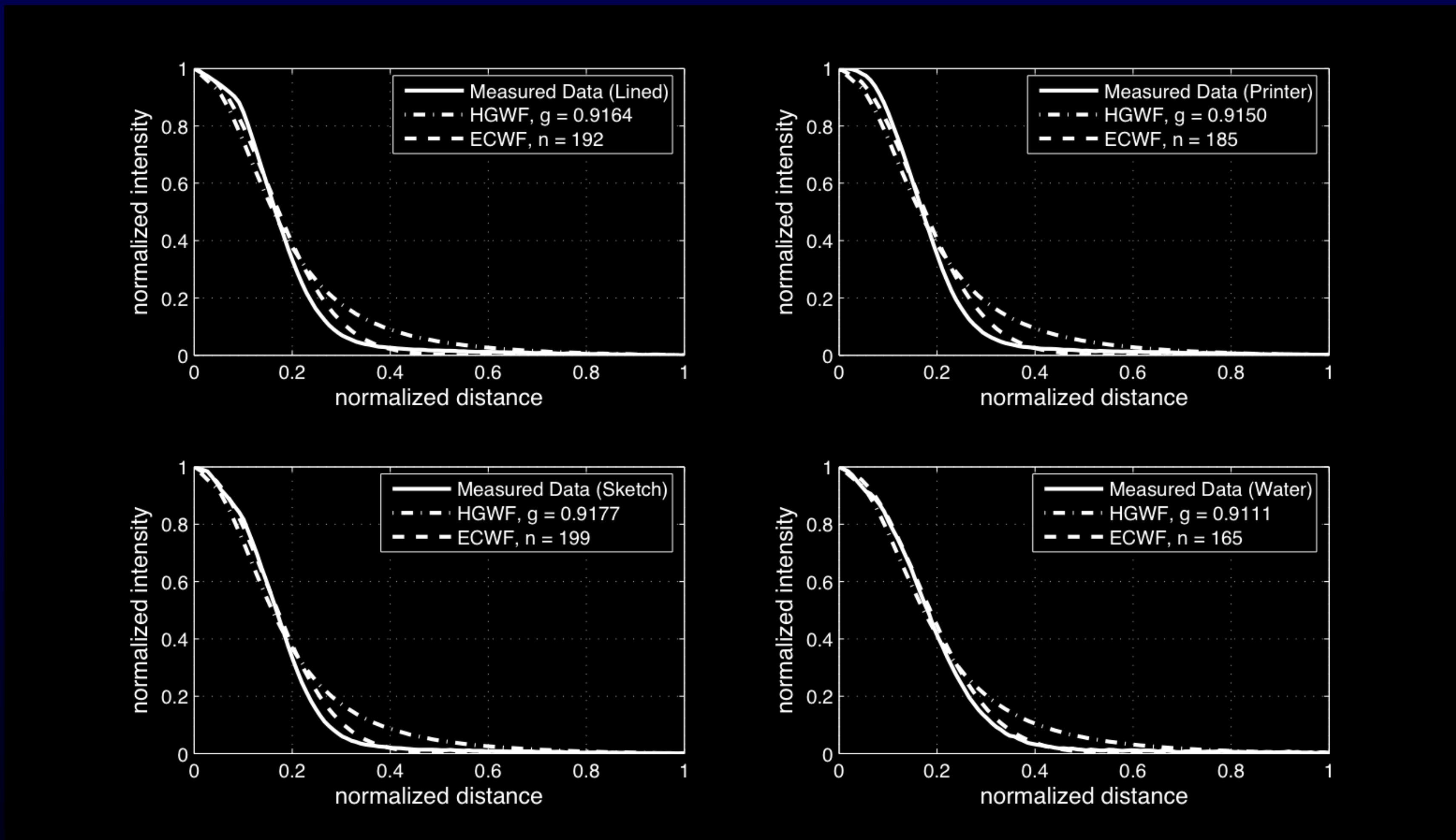
- Experiments involving different types of paper



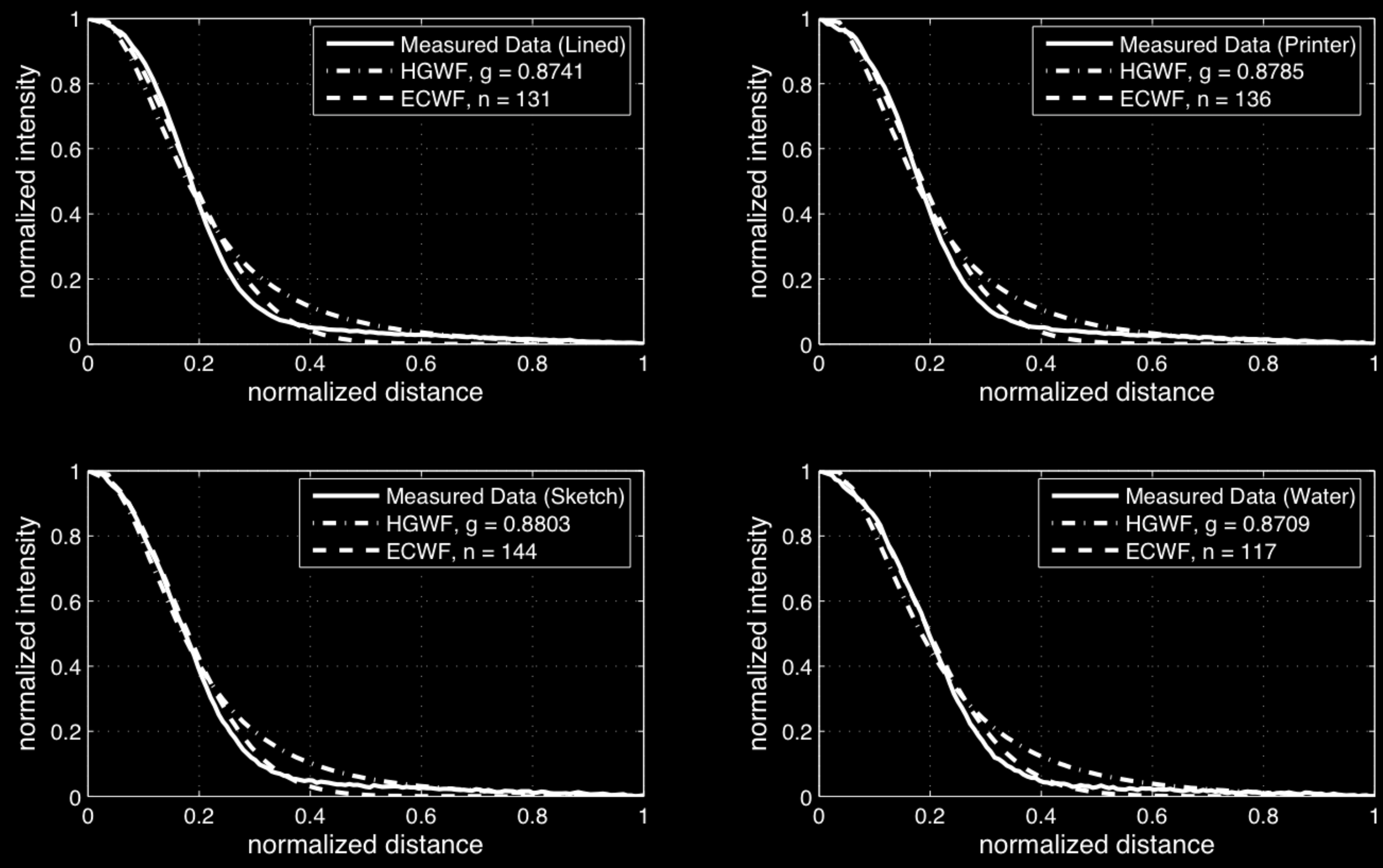



**(Chen and Baranoski, Optics Express 2008)**

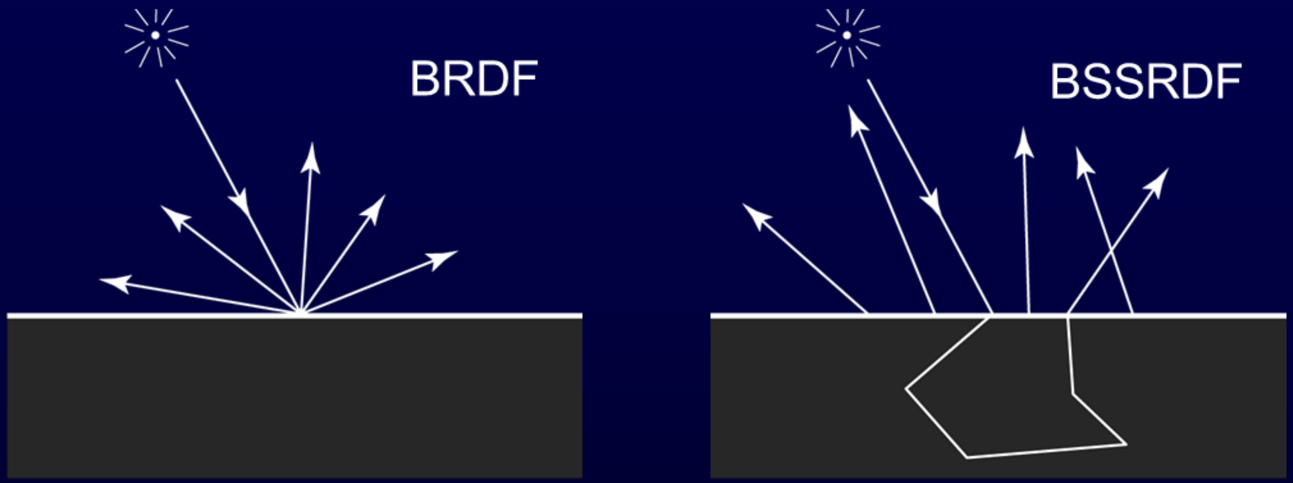
# Comparison of Measured (at 543nm) and Simulated Scattering Data for Paper



# Comparison of Measured (at 633nm) and Simulated Scattering Data for Paper



- Does position matter?

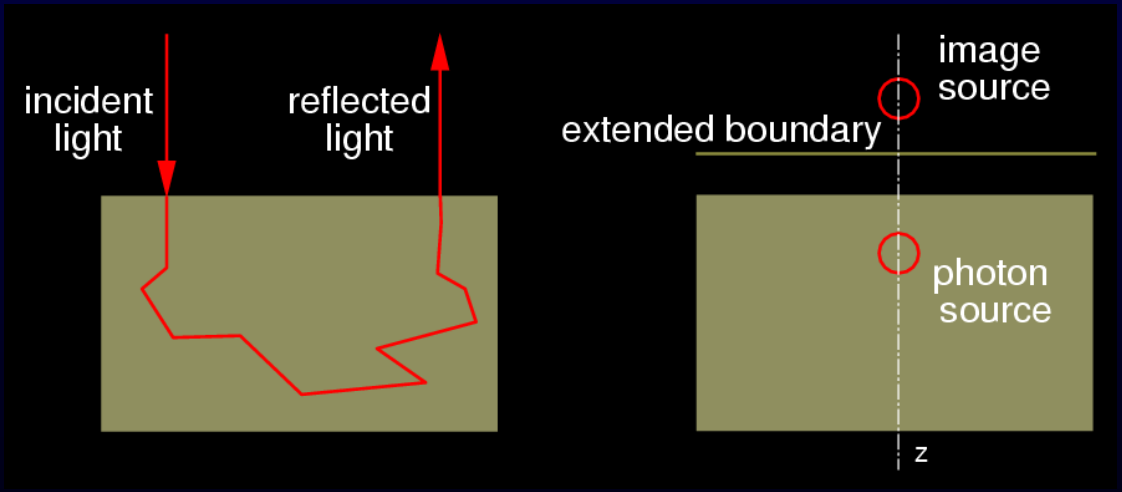



  - Models based on the Diffusion theory have been employed to address this issue

- Example: dipole model proposed by Farell and Patterson (1992)

  - ❖ accounts for the dependence of the diffuse reflectance on the radial distance from the light source

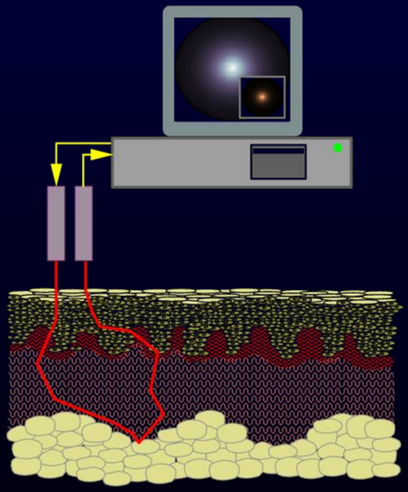
  - ❖ incorporates a photon dipole source in order to satisfy the tissue boundary conditions



- Applicability of the diffusion theory

  - ❖ recall that the theory provides a **poor** approximation when the absorption coefficient of a turbid medium is **not** significantly smaller than the scattering coefficient

  - ❖ it is mostly used in biomedical applications involving lasers and mammalian tissues



# Outline

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- ✓ Simulation Approaches
- ✓ Level of Abstraction
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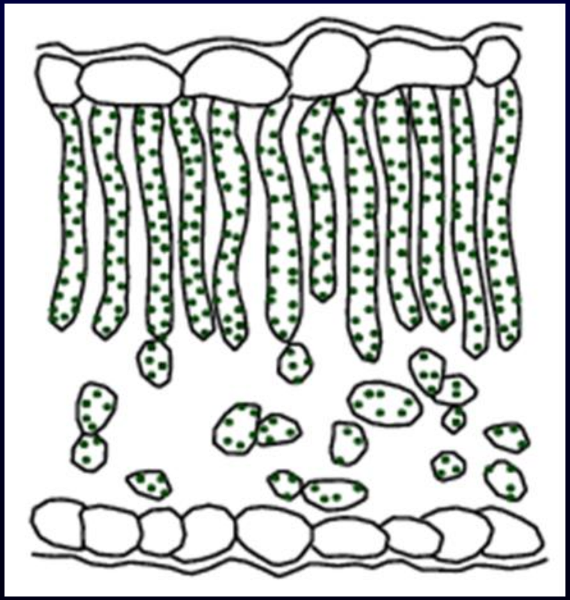
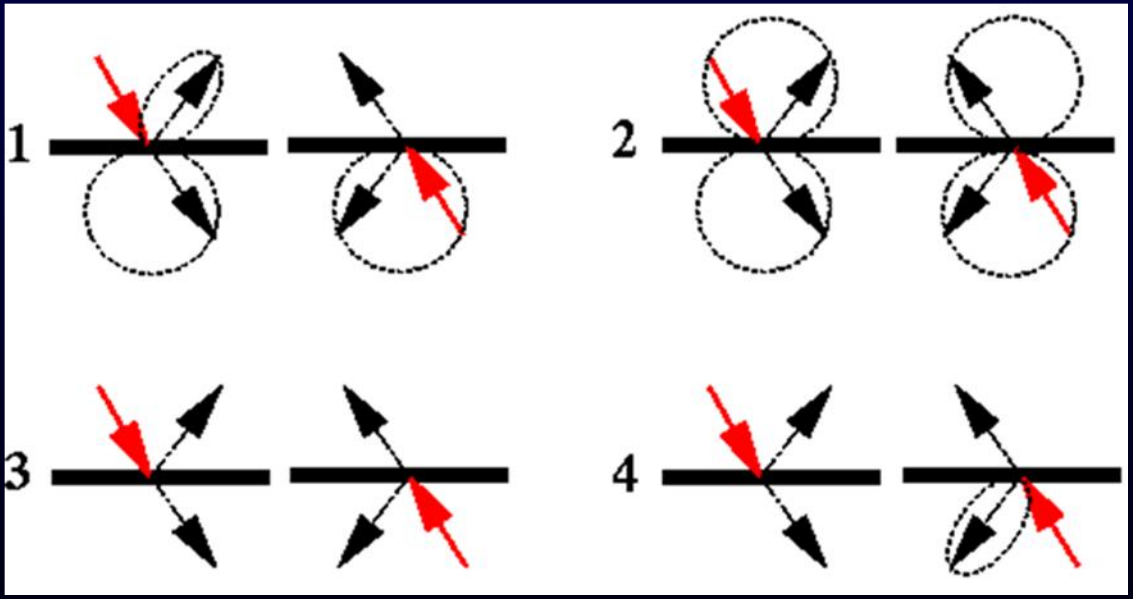
# Design Evolution

- Application driven evolution
  - Example: spectral responses of plant leaves

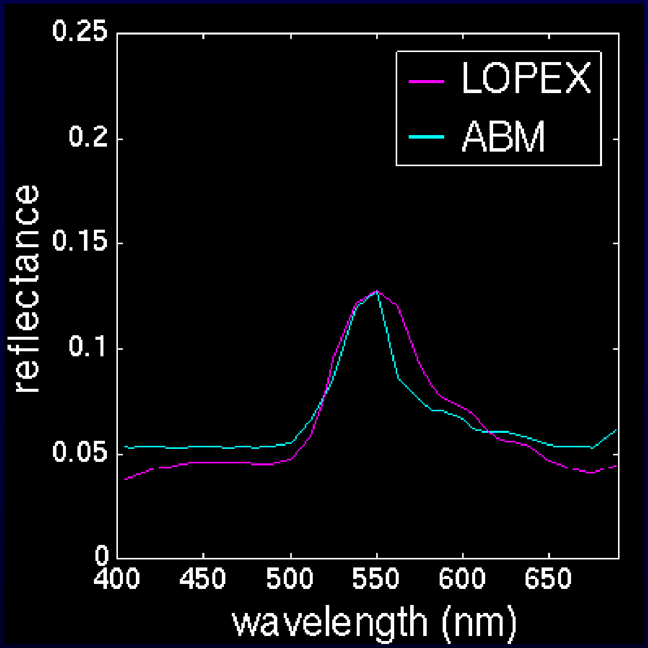
Cross-Section

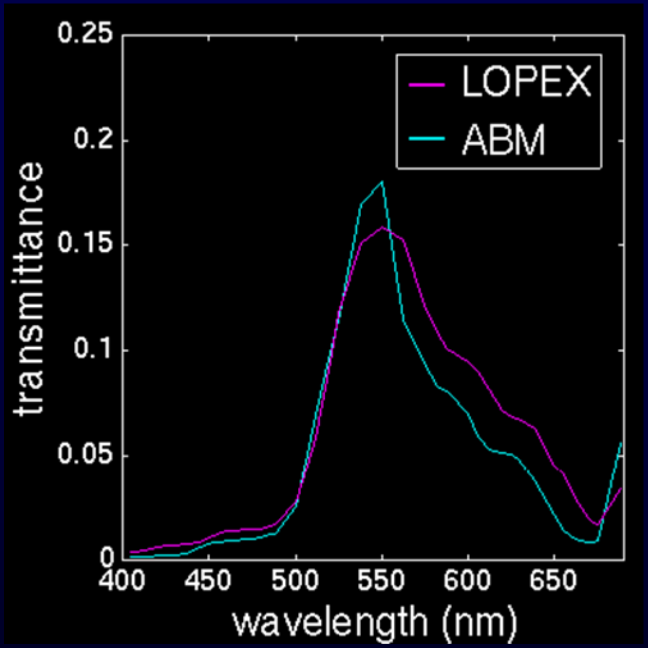


Layered ABM Model for Plant Leaves

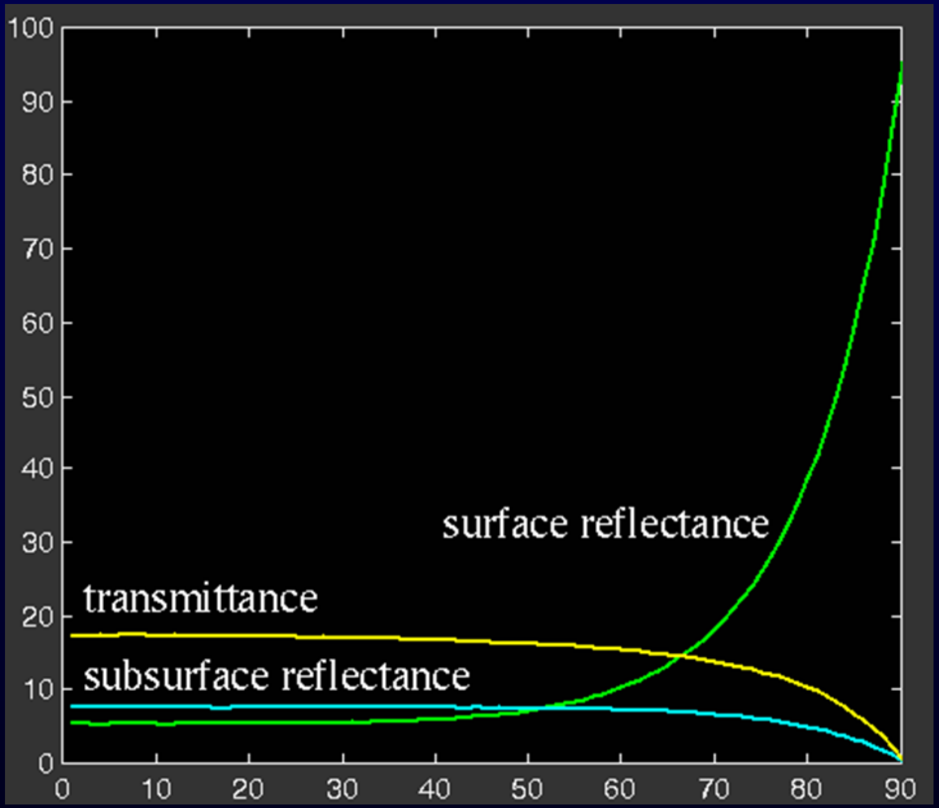


# Measured (LOPEX) and Modeled (ABM) Soybean Spectral Signatures



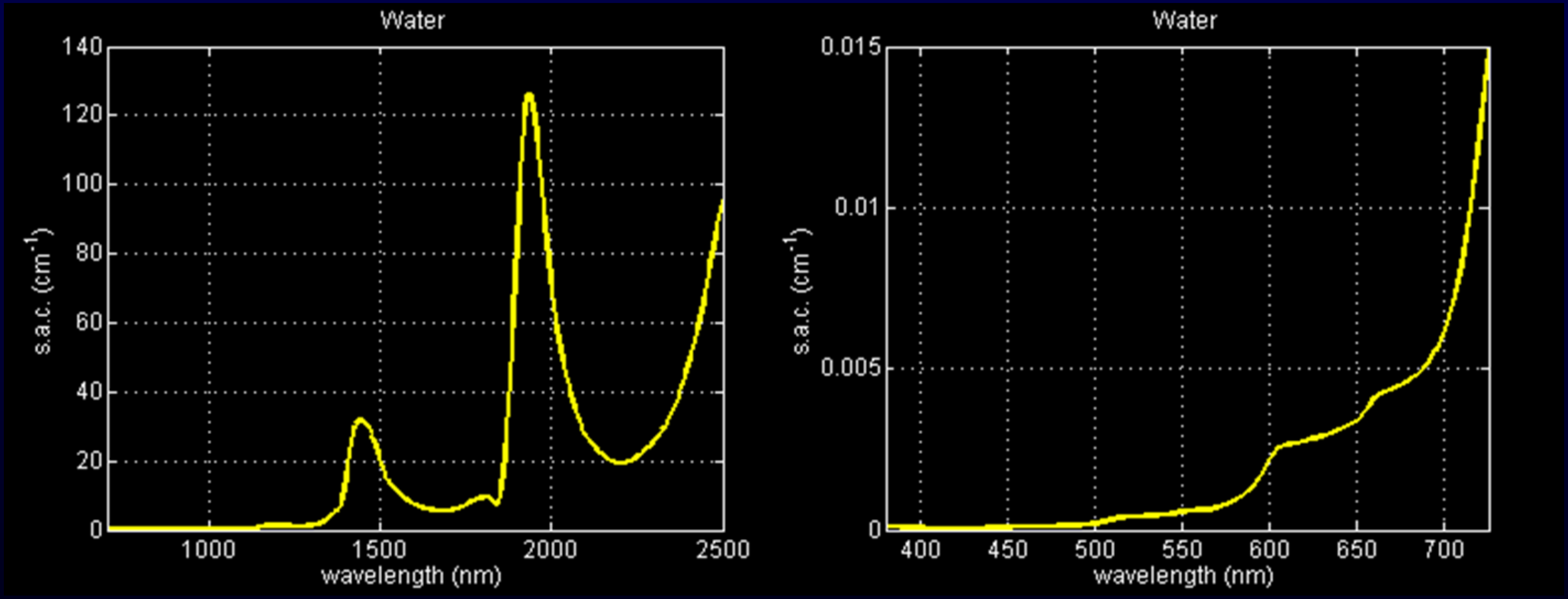
# Modeled (ABM) Soybean Spectral Curves




%

angle of incidence

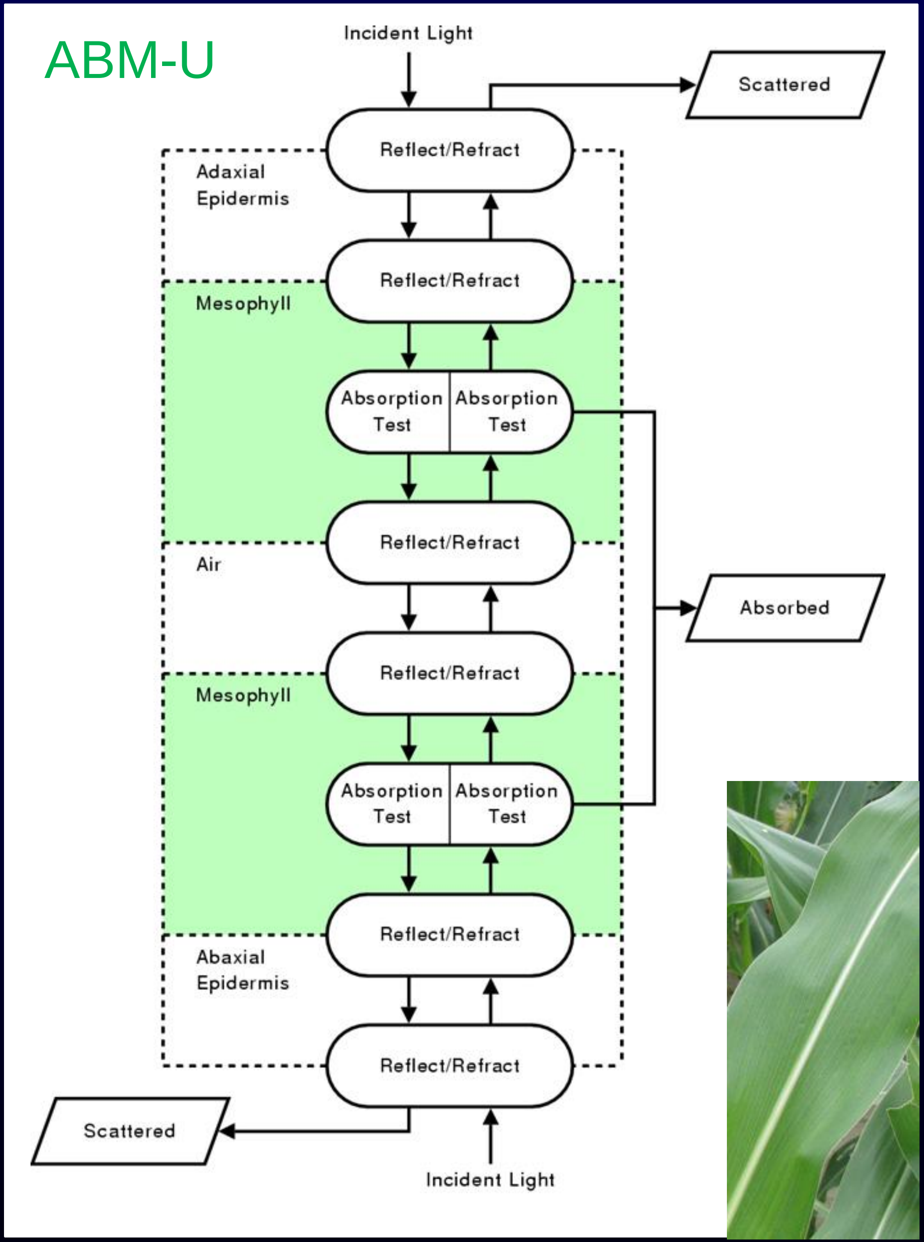
- How about spectral signatures in the infrared domain?
- What is the major absorber in this domain?

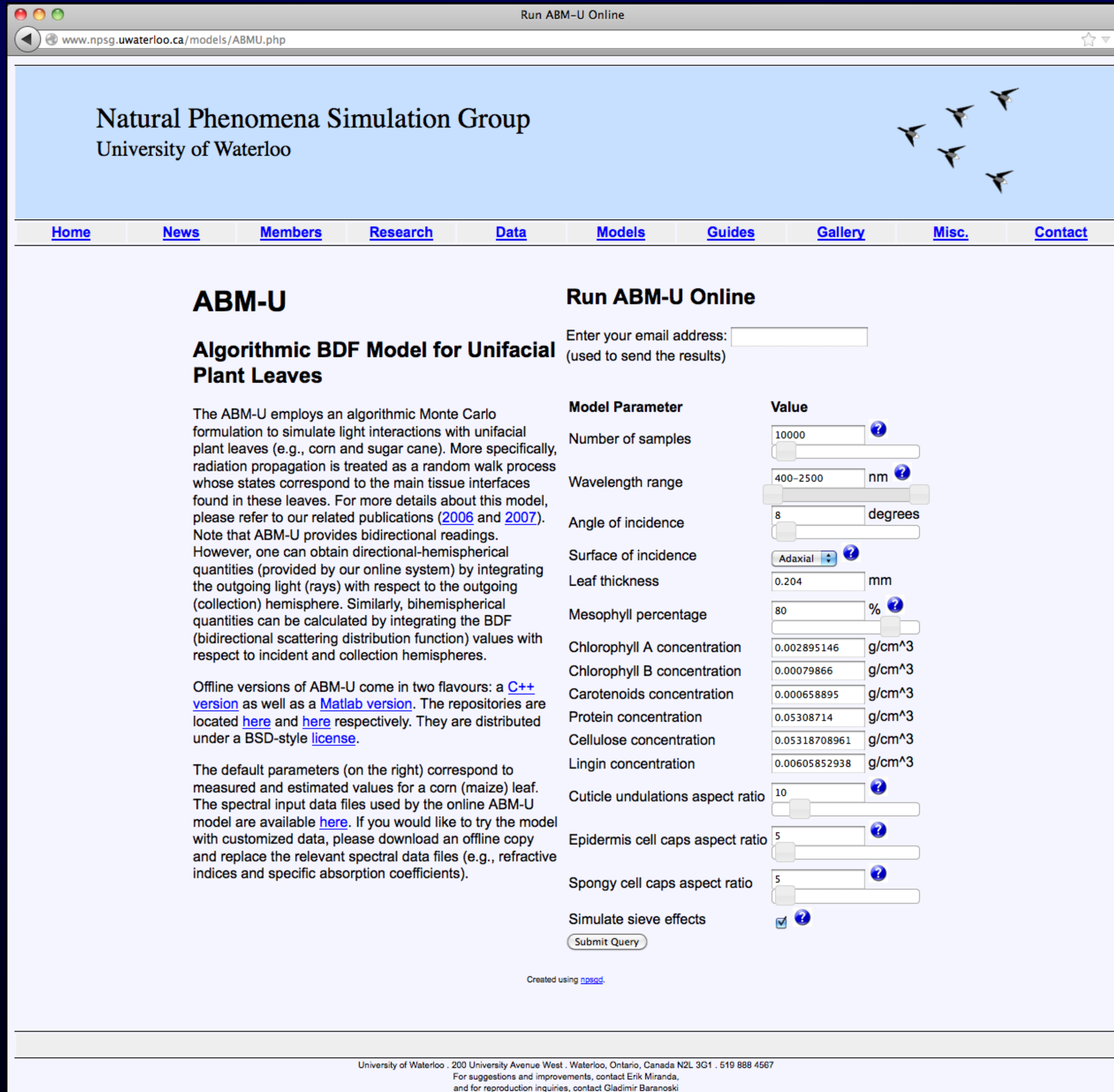


- How about structural differences between unifacial and bifacial plant leaves?

↓ ABM-U

↓ ABM-B


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


Run ABM-U Online

www.npsg.uwaterloo.ca/models/ABMU.php

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# 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 BDF (bidirectional scattering distribution function) values with respect to incident and collection hemispheres.

Offline versions of ABM-U come in two flavours: a C++ version as well as a Matlab version. The repositories are located here and here respectively. They are distributed under a BSD-style license.

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. If you would like to try the model with customized data, please download an offline copy and replace the relevant spectral data files (e.g., refractive indices and specific absorption coefficients).

## Run ABM-U Online

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

| Model Parameter | Value |
|---|---|
| Number of samples | 10000 |
| Wavelength range | 400-2500 nm |
| Angle of incidence | 8 degrees |
| Surface of incidence | Adaxial |
| Leaf thickness | 0.204 mm |
| Mesophyll percentage | 80 % |
| Chlorophyll A concentration | 0.002895146 g/cm^3 |
| Chlorophyll B concentration | 0.00079866 g/cm^3 |
| Carotenoids concentration | 0.000658895 g/cm^3 |
| Protein concentration | 0.05308714 g/cm^3 |
| Cellulose concentration | 0.05318708961 g/cm^3 |
| Lingin concentration | 0.00605852938 g/cm^3 |
| Cuticle undulations aspect ratio | 10 |
| Epidermis cell caps aspect ratio | 5 |
| Spongy cell caps aspect ratio | 5 |
| Simulate sieve effects | ☑ |

Submit Query

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Run ABM-B Online

www.npsg.uwaterloo.ca/models/ABMB.php

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# ABM-B

## Algorithmic BDF Model for Bifacial Plant Leaves

The ABM-B employs an algorithmic Monte Carlo formulation to simulate light interactions with bifacial plant leaves (e.g., soybean and maple). 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-B 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 BDF (bidirectional scattering distribution function) values with respect to incident and collection hemispheres.

Offline versions of ABM-B come in two flavours: a C++ version as well as a Matlab version. The repositories are located here and here respectively. They are distributed under a BSD-style license.

The default parameters (on the right) correspond to measured and estimated values for a soybean leaf. The spectral input data files used by the online ABM-B model are available here. If you would like to try the model with customized data, please download an offline copy and replace the relevant spectral data files (e.g., refractive indices and specific absorption coefficients).

## Run ABM-B Online

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

| Model Parameter | Value |
|---|---|
| Number of samples | 10000 |
| Wavelength range | 400-2500 nm |
| Angle of incidence | 8 degrees |
| Surface of incidence | Adaxial |
| Leaf thickness | 0.166 mm |
| Mesophyll percentage | 50 % |
| Chlorophyll A concentration | 0.0039775 g/cm^3 |
| Chlorophyll B concentration | 0.0011613 g/cm^3 |
| Carotenoids concentration | 0.0011323 g/cm^3 |
| Protein concentration | 0.078059 g/cm^3 |
| Cellulose concentration | 0.0377565 g/cm^3 |
| Lingin concentration | 0.0107441 g/cm^3 |
| Cuticle undulations aspect ratio | 5 |
| Epidermis cell caps aspect ratio | 5 |
| Palisade cell caps aspect ratio | 1 |
| Spongy cell caps aspect ratio | 5 |
| Simulate sieve effects | ☑ |

Submit Query

Created using npsgd.

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For suggestions and improvements, contact Erik Miranda,
and for reproduction inquiries, contact Gladimir Baranoski

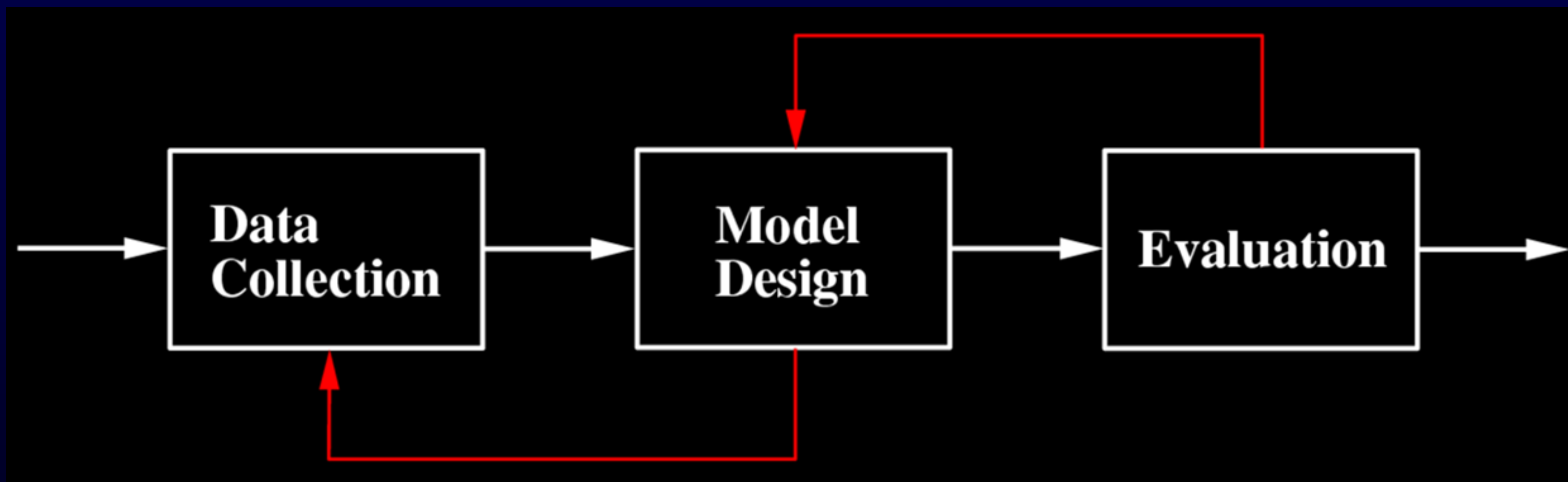
- Are the phenomena to be modeled fully understood?
- What if they are not?

# Outline

- ✓ Drawing Board
- ✓ Simulation Approaches
- ✓ Level of Abstraction
- ✓ Design Evolution
- ❑ Iterative Refinement

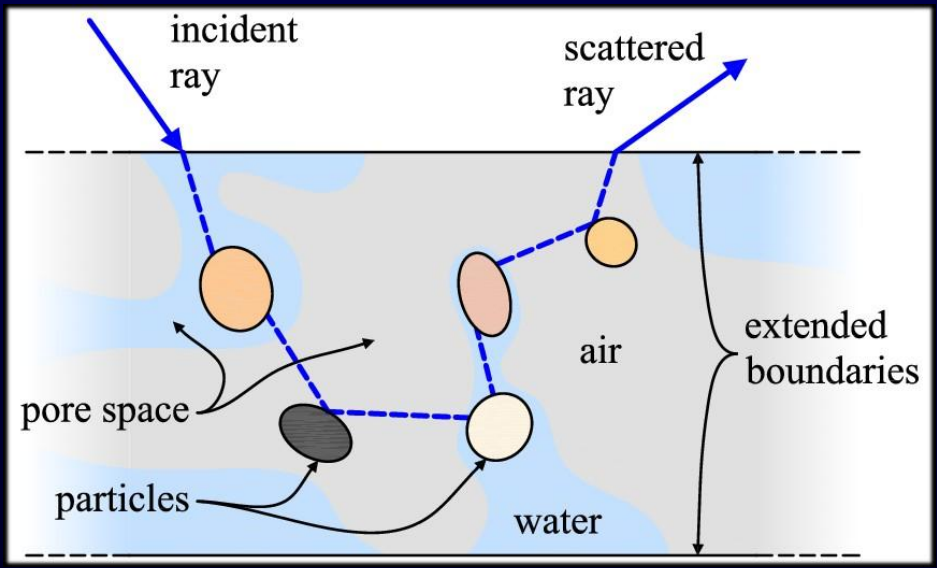
# Iterative Refinement

- A model development framework is usually non-linear

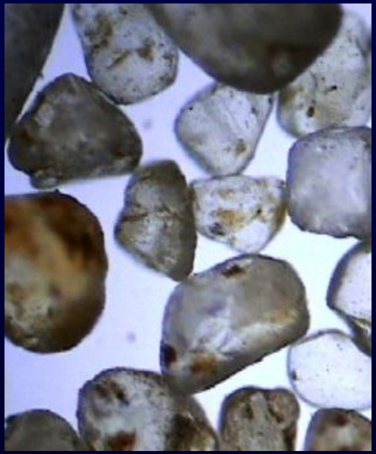


## ➢ Key insights can be obtained through *in situ* observations …

- Example: SPLITS simulations

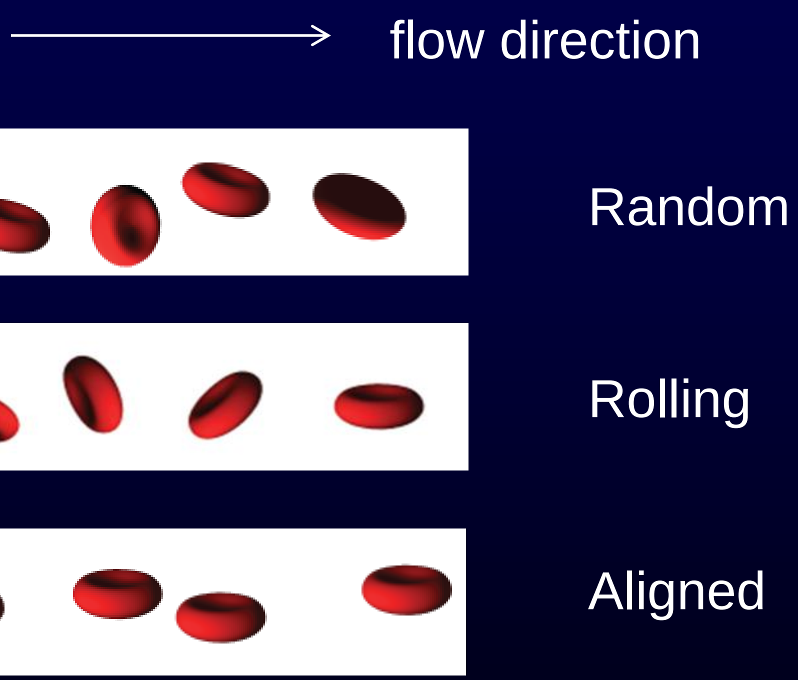






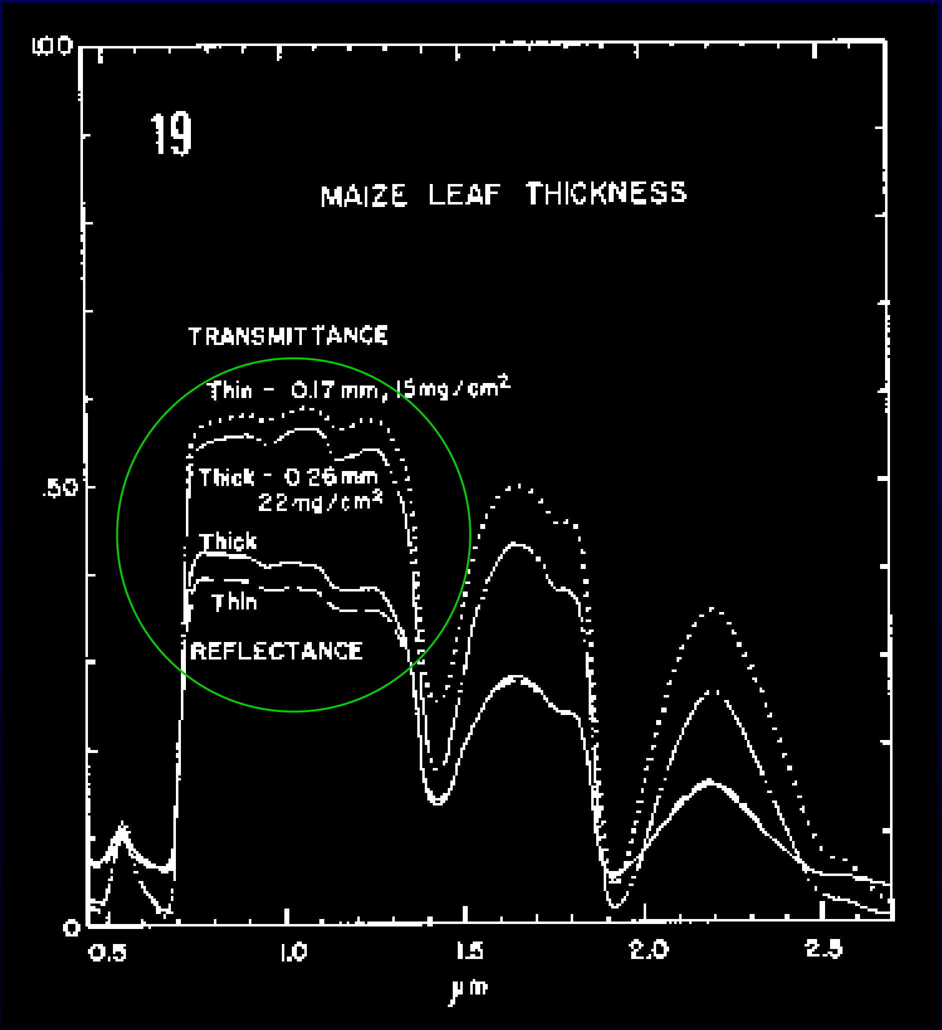
## ➢ … and qualitative comparisons with experimental data

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



- Example: spectral responses of unifacial plant leaves

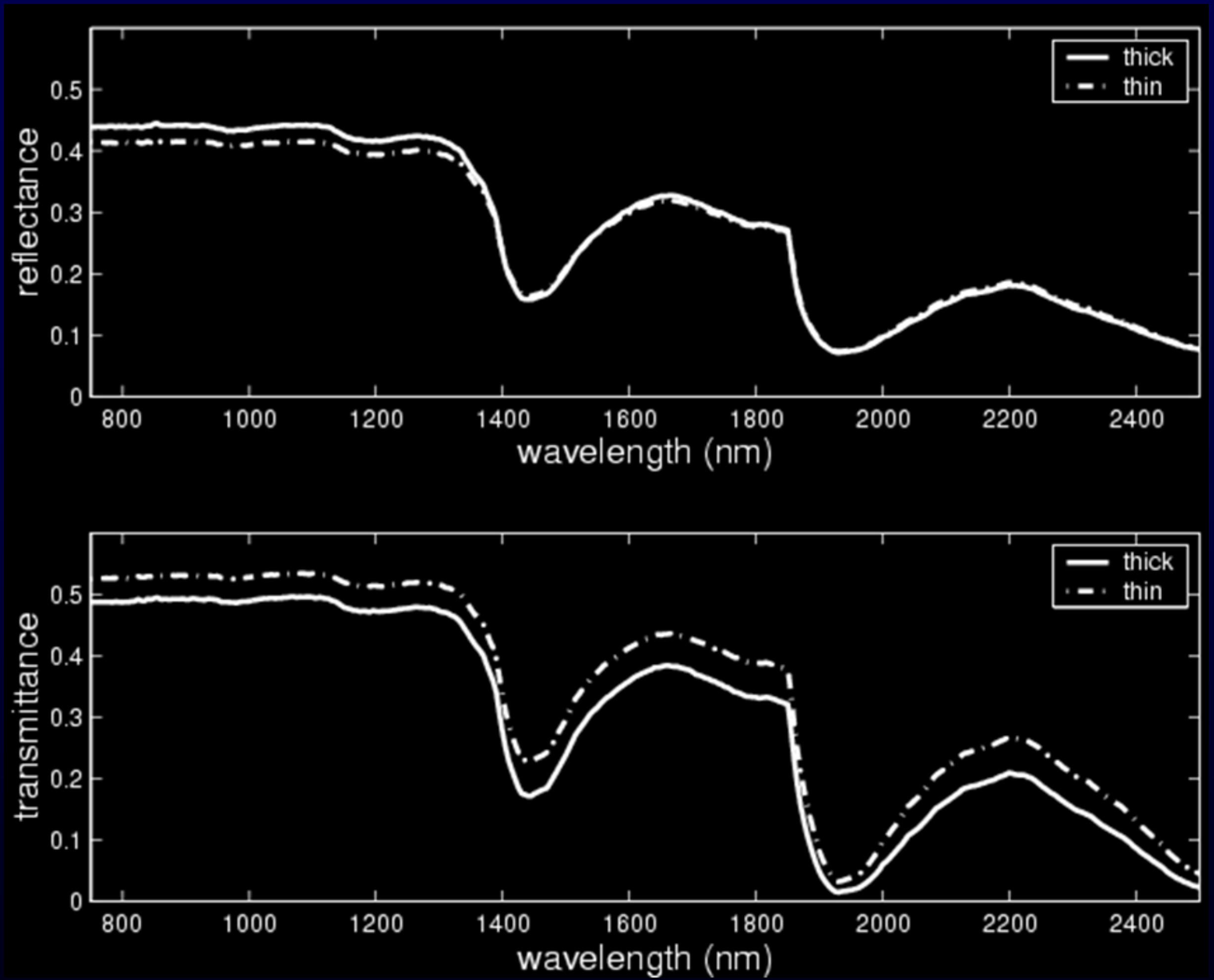
Measured Corn Spectral Curves




(Woolley, Plant Physiology 1971)

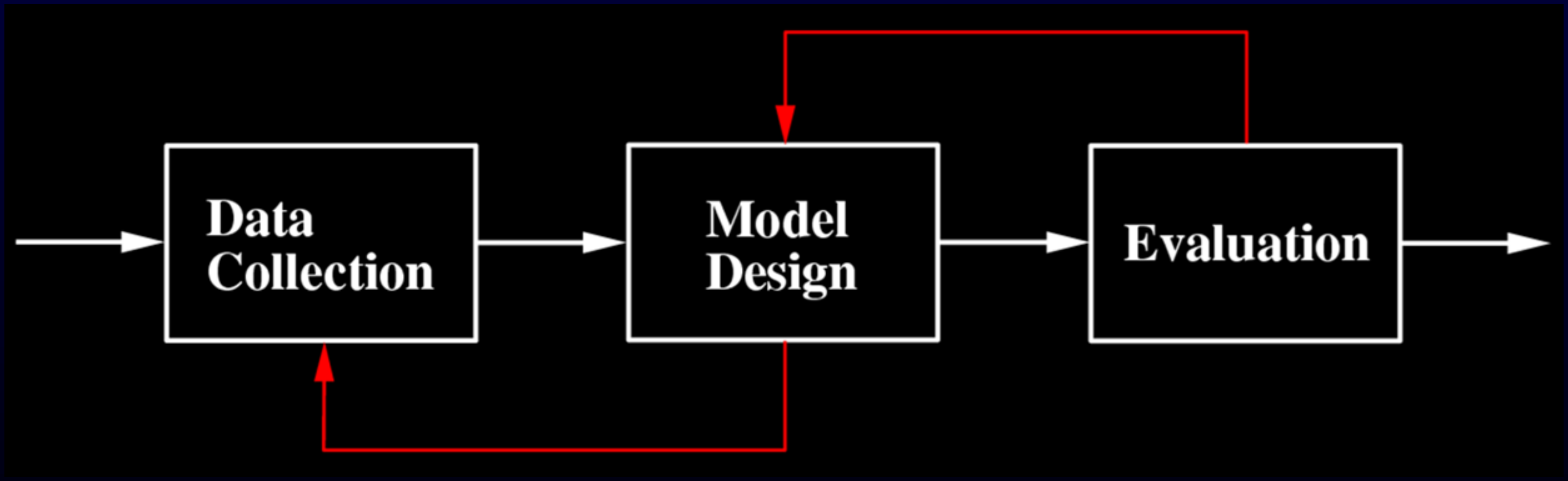
- … and qualitative comparisons with experimental data

Modeled (ABM-U) Corn Spectral Curves

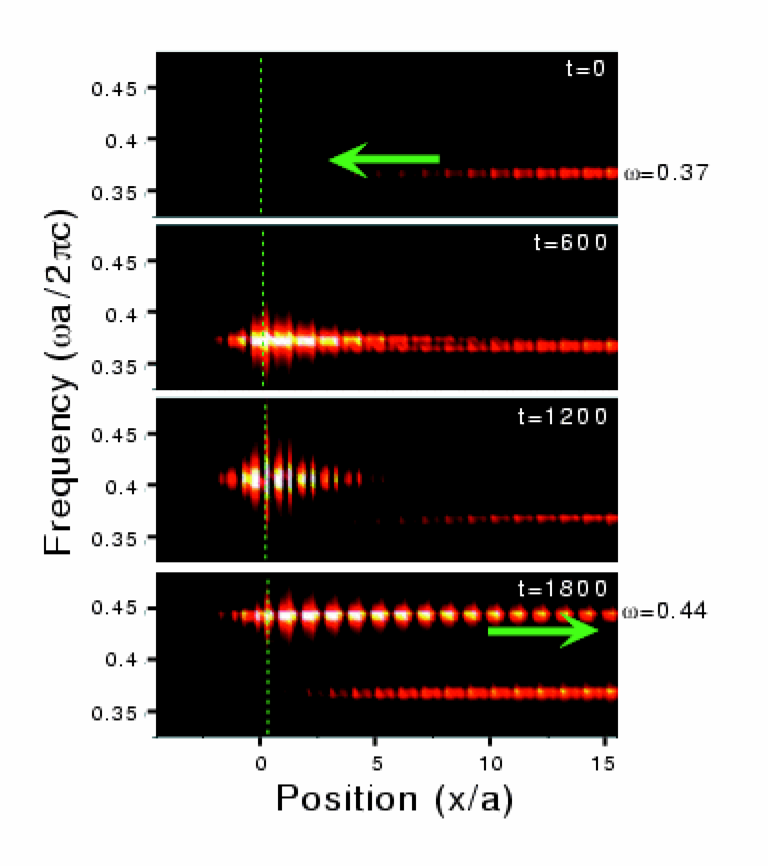


## ➢ Interaction with experimental investigation

- 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 color of shock waves in photonic crystals”
Reed *et al.*, Physical Review Letters, 2003



"The most exciting phrase to hear in science,
the one that heralds new discoveries,
is not 'Eureka',
but 'That's funny…'"

Isaac Asimov

*This concludes Lecture 3!*

*Thanks!*

*Questions?*

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