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

Lecture Series

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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

Evaluation: The Key for Assessing “Real” Contributions

Lecture 4

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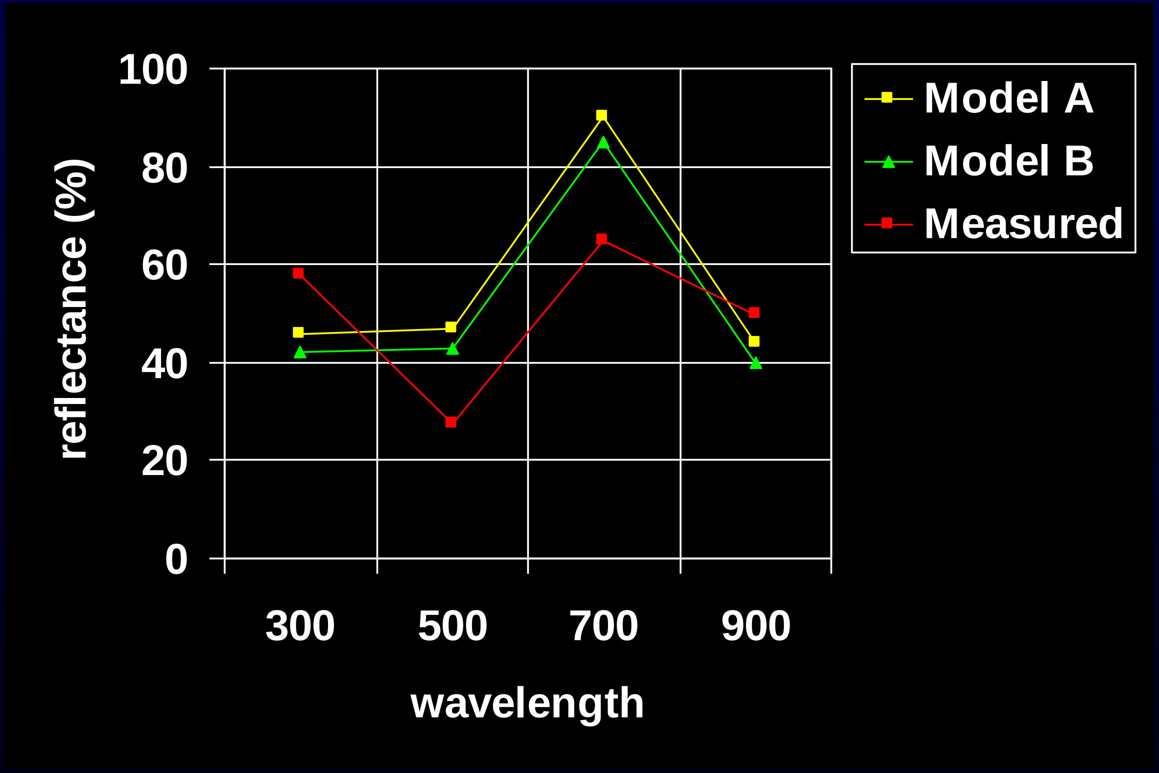
Outline

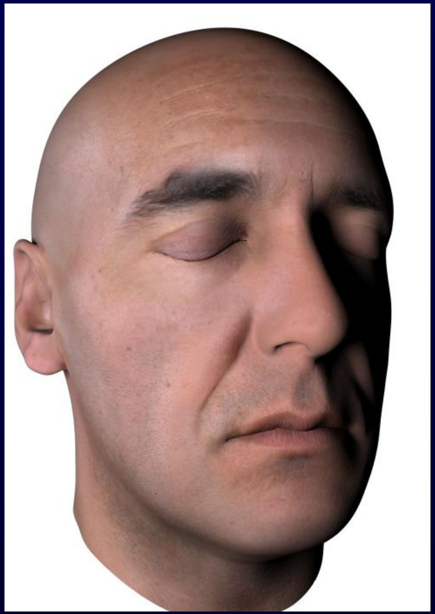
- Parallel Comparisons
- Quantitative Comparisons
- Qualitative Comparisons
- Accuracy vs. Efficiency
- Reproducibility and Transparency

Parallel Comparisons

- Comparisons with other models based on similar approaches



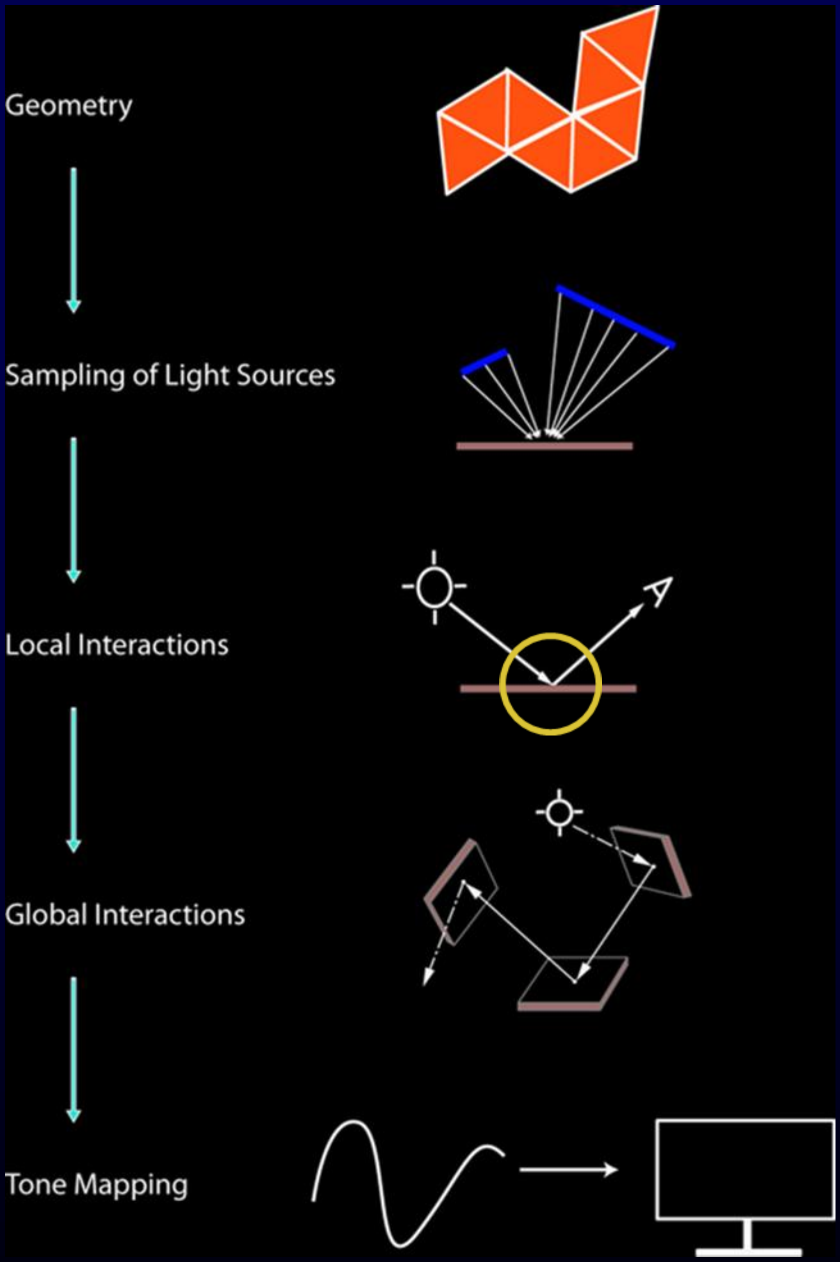
➢ Visual Inspection



BioSpec

Lambertian

Image Synthesis Pipeline



- Geometry and texture maps may bias the comparisons

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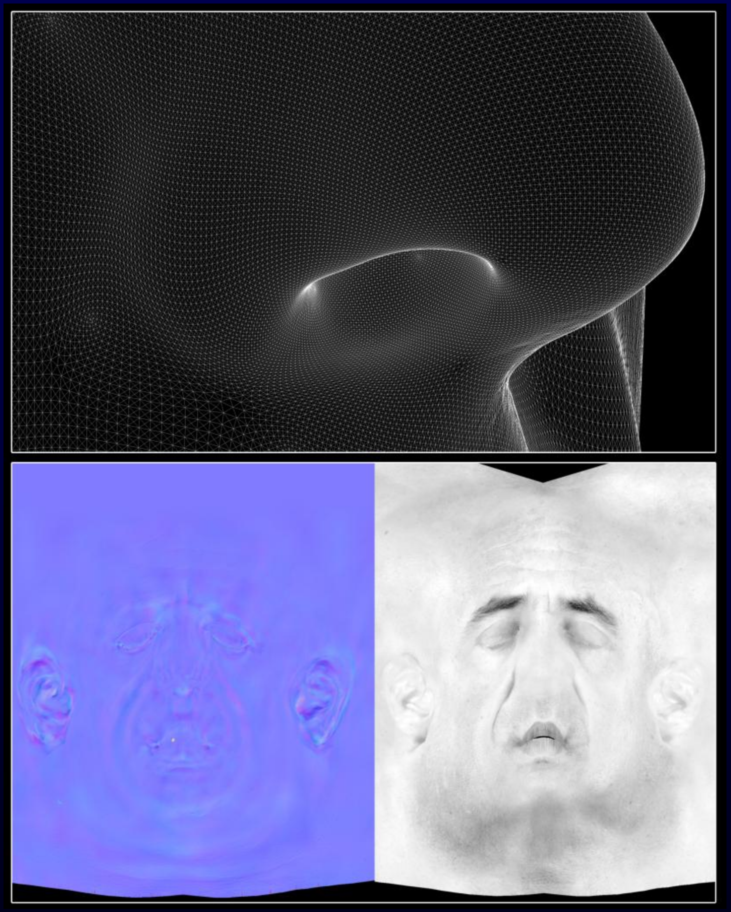


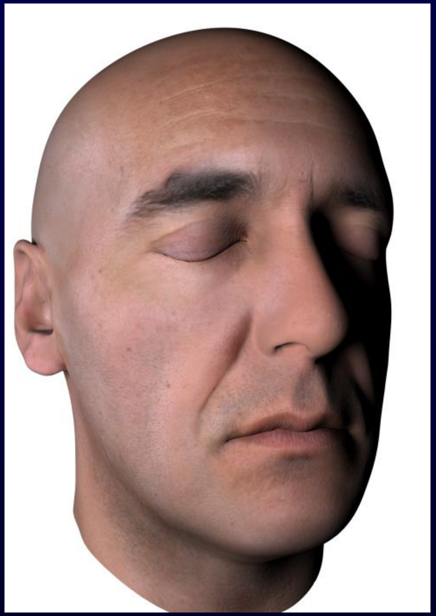
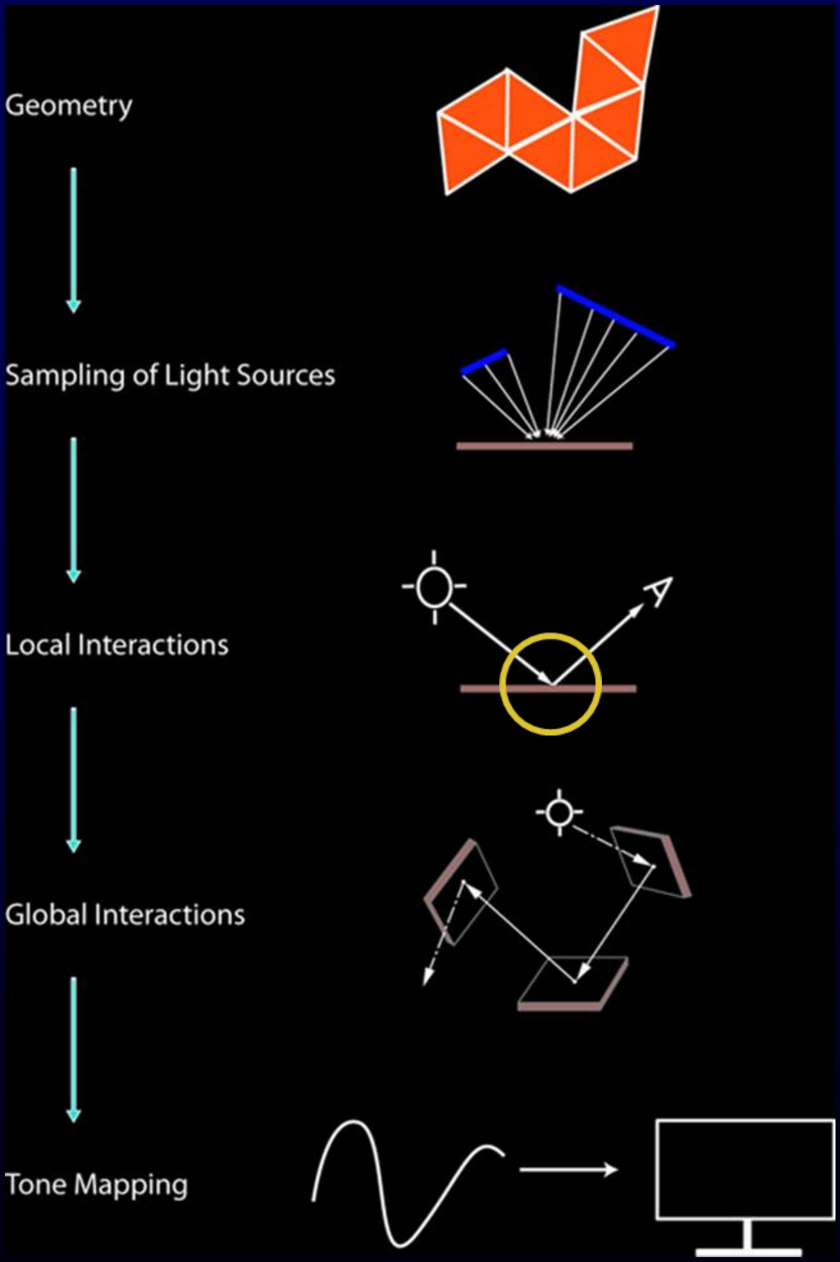
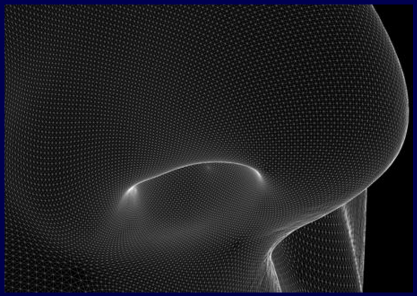
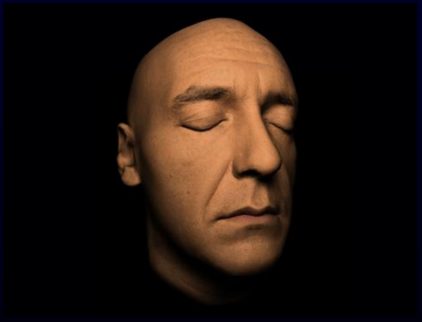


Image Synthesis Pipeline



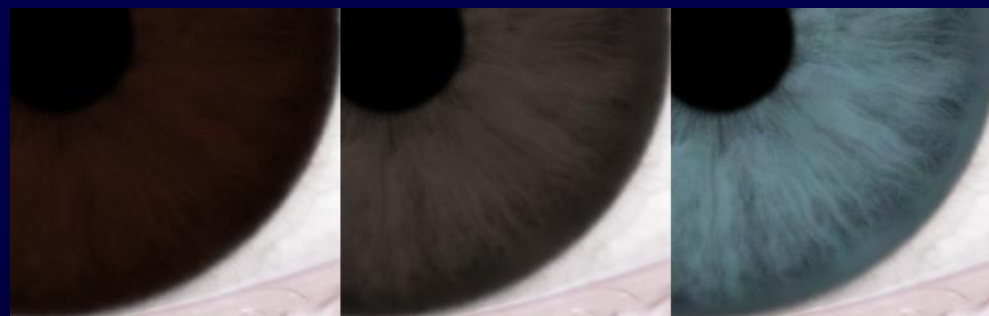


BioSpec

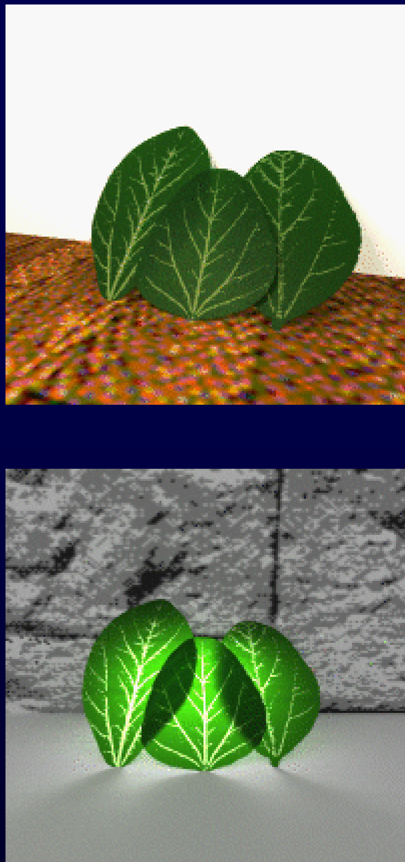


- Tone (color) reproduction issues may also affect the results

CIE-1931 Chromaticity Coordinates



SMPTE Chromaticity Coordinates



ABM

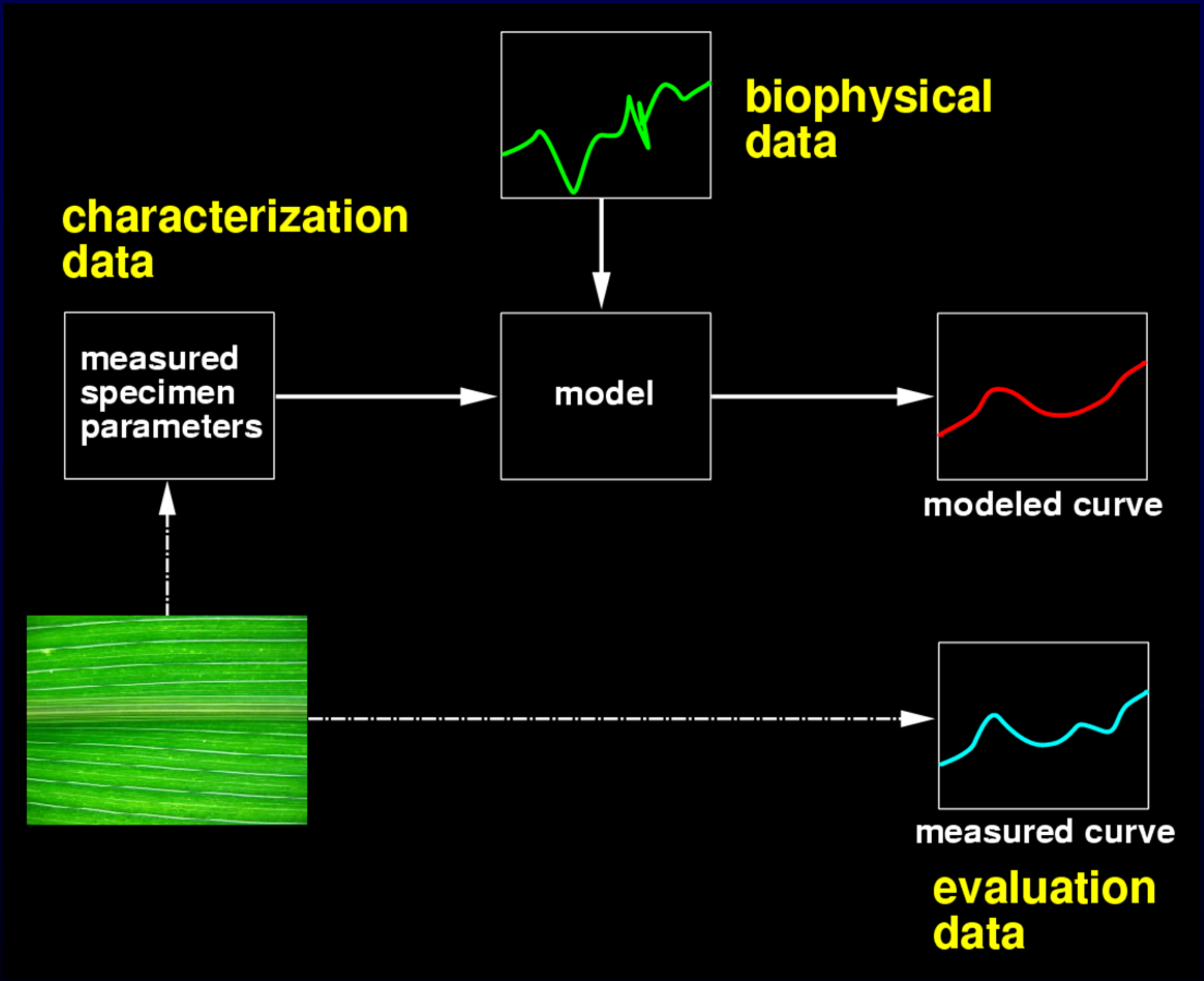
“Artistic” Colors

ABM-B

Outline

- ✓ Parallel Comparisons
- ❑ Quantitative Comparisons
- ❑ Qualitative Comparisons
- ❑ Accuracy vs. Efficiency
- ❑ Reproducibility and Transparency

Quantitative Comparisons



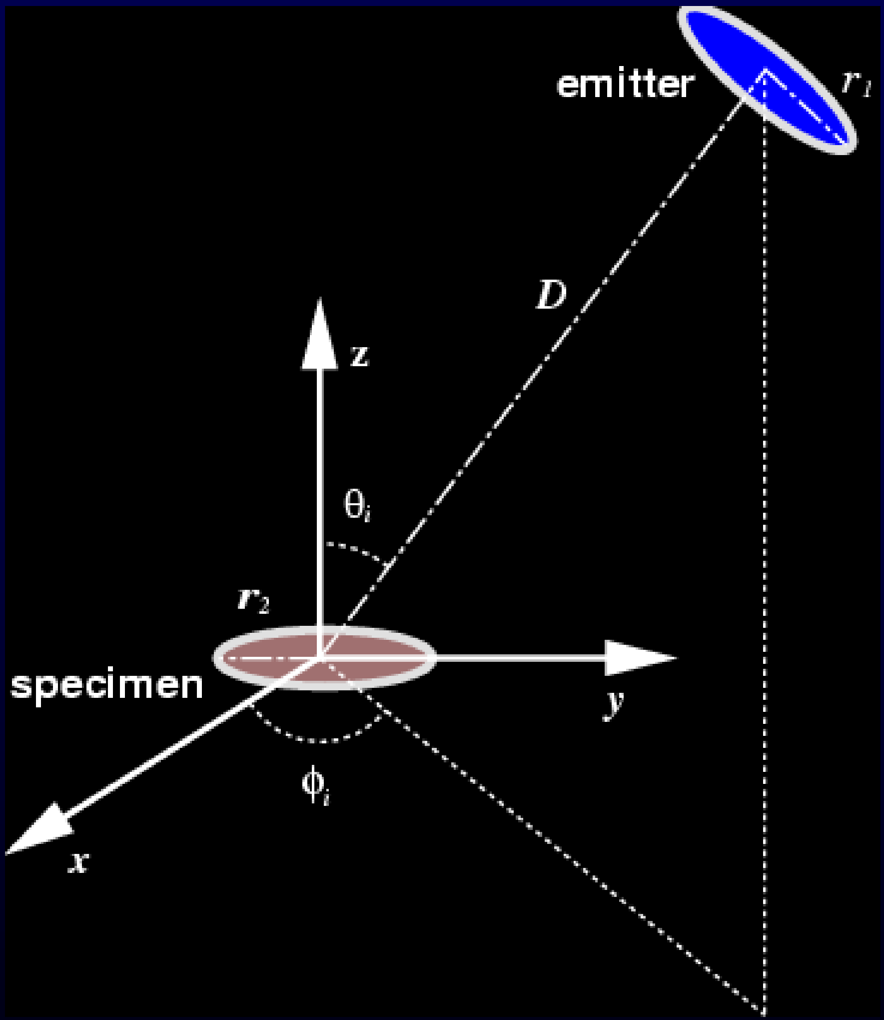
- Reproduction of measurement (experimental) conditions as faithfully as possible:

  - Specimen’s characterization data
  - Incidence and viewing geometries
  - Actual devices’ accuracy and precision
  - Proper implementation of virtual measurement devices

- Virtual spectrophotometer

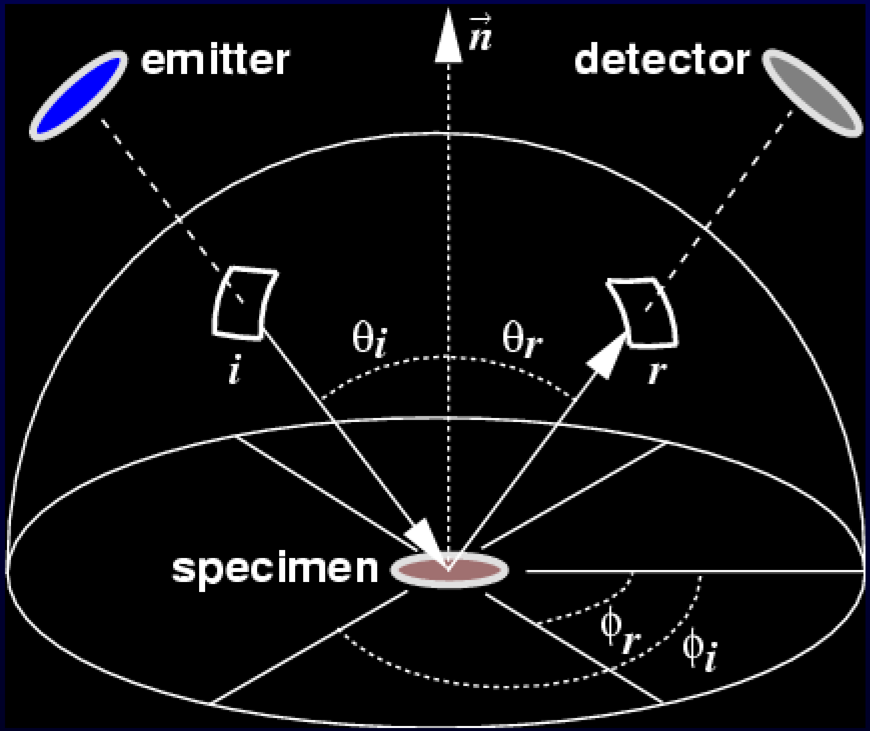
  - Considering N rays shot toward the specimen, if m rays are reflected toward the upper hemisphere, then the directional-hemispherical reflectance is given by:

$$\rho(\lambda,\vec{\omega}_i,\Omega_r) = \frac{m}{N}$$



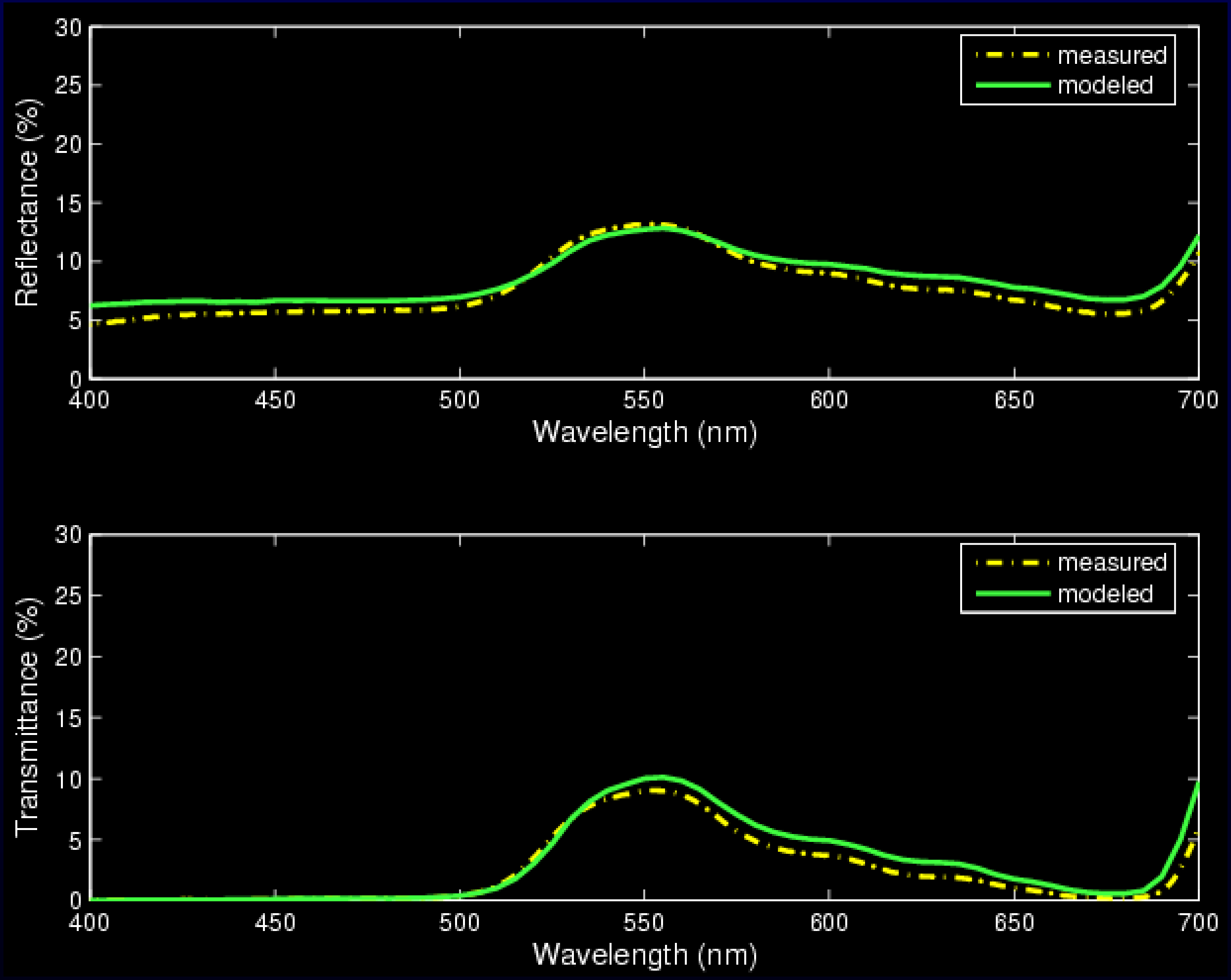
- Virtual goniophotometer
  - Considering N rays shot toward the specimen (direction i), if m_r rays are reflected (direction r), then the BRDF is given by:

$$f_r(\lambda, \vec{\omega}_i, \vec{\omega}_r) = \frac{m_r}{N\, \vec{\omega}_r^{\,p}}$$



- “Direct” comparisons with measured data

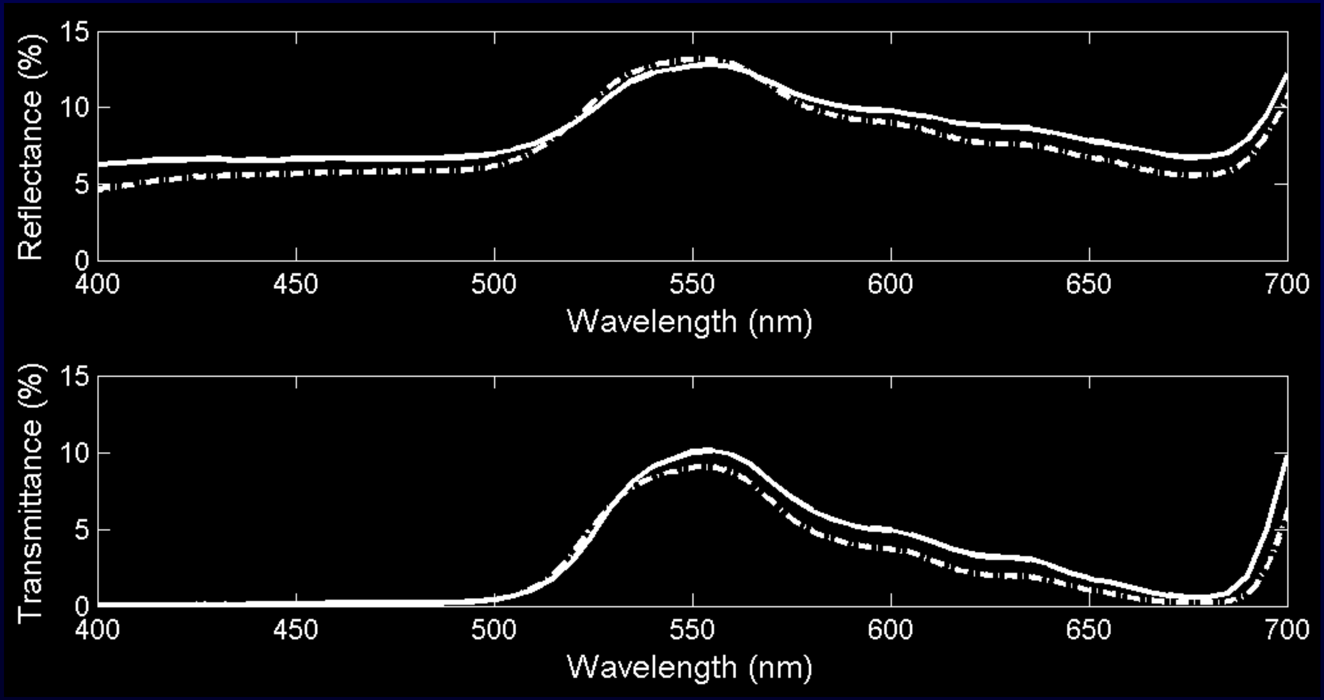
Modeled (ABM-U) and Measured (LOPEX) Spectral Signatures



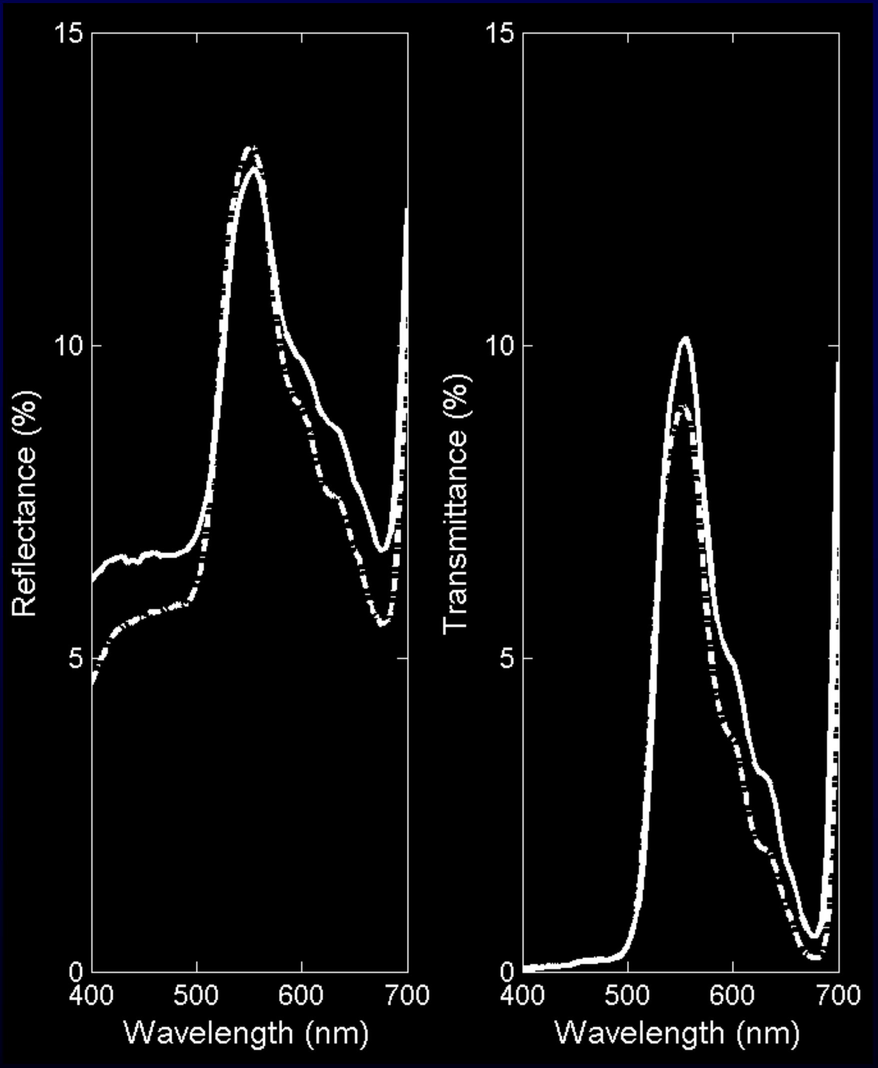
LOPEX

ABM-U

- Is this a “good” agreement?



- Are the curves really close?



- Can we use an error metrics? Which one?

  - ❖ How about RMS errors?
  - ❖ reflectance curve < 0.0096
  - ❖ transmittance curve < 0.0093
  - ❖ Are these values “good” or “bad”?

< 0.03

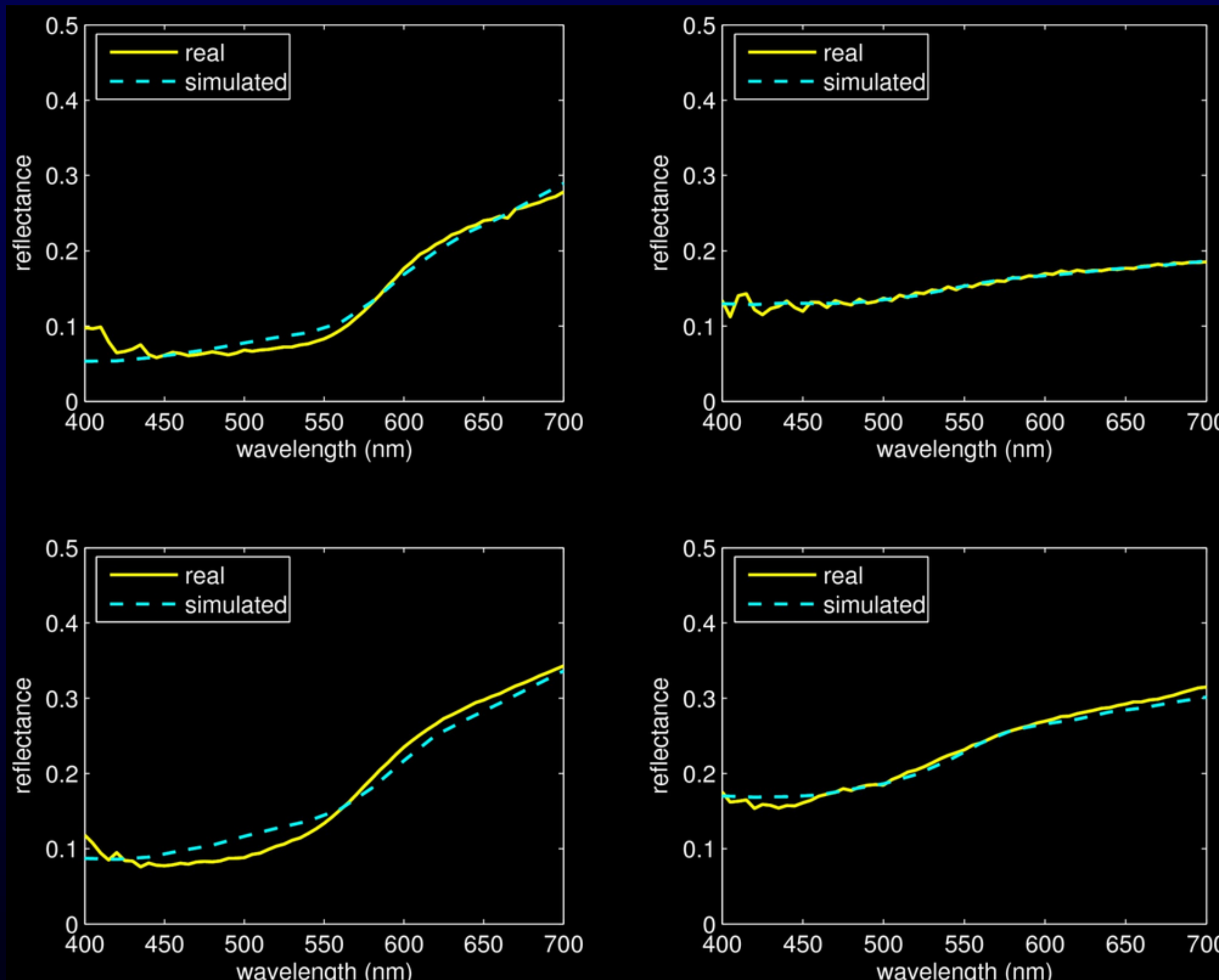
➢ What if exact values for key material parameters are missing?

- We can search the parameter spaces for the best matches
- Important: to keep the parameter values within actual ranges
- We should specify the procedure used to select parameter values
    - 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

Outline

- ✓ Parallel Comparisons
- ✓ Quantitative Comparisons
- ❑ Qualitative Comparisons
- ❑ Accuracy vs. Efficiency
- ❑ Reproducibility and Transparency

Qualitative Comparisons

- Based on visual observations of actual phenomena

ABM

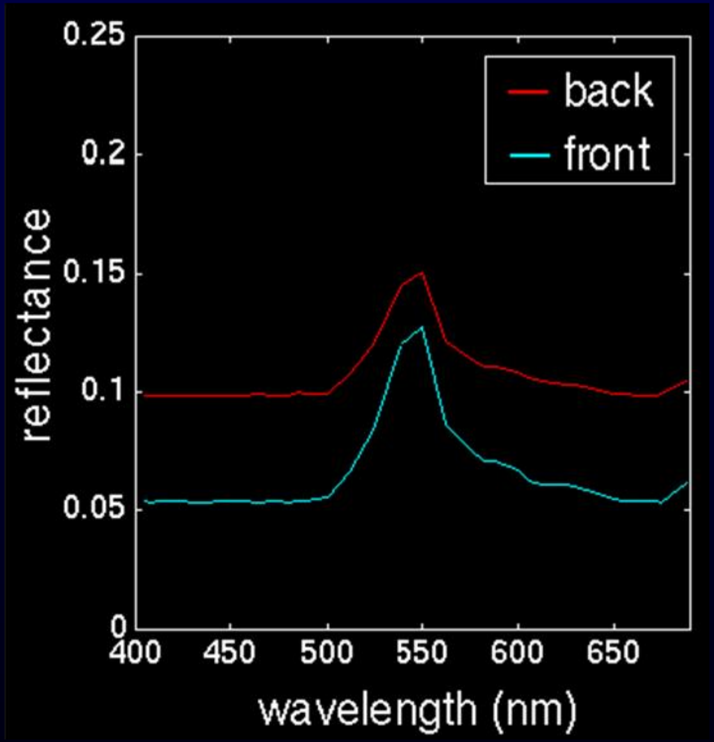
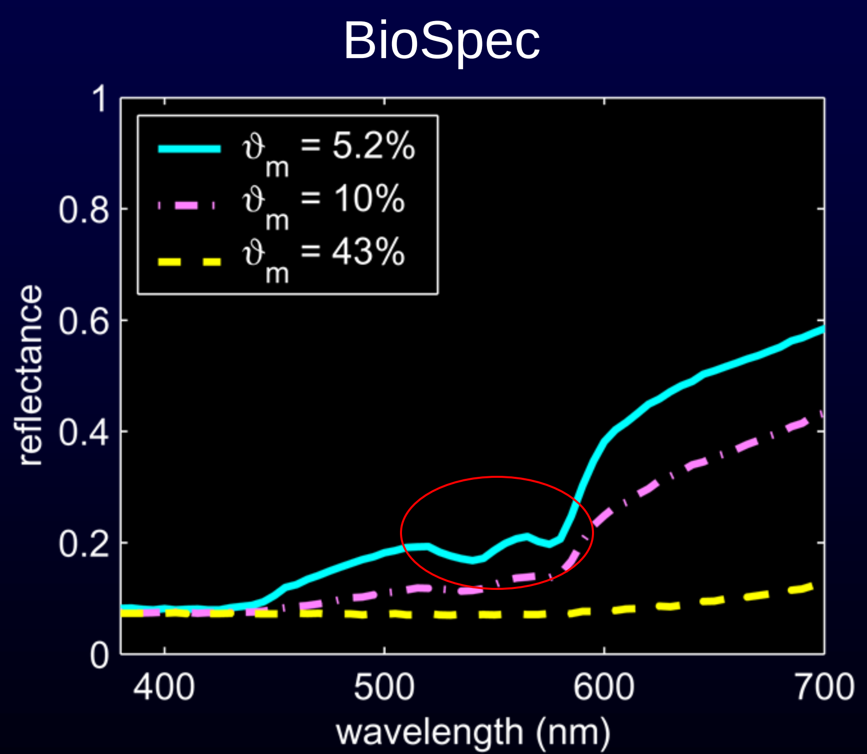


Photo of Soybean Leaves

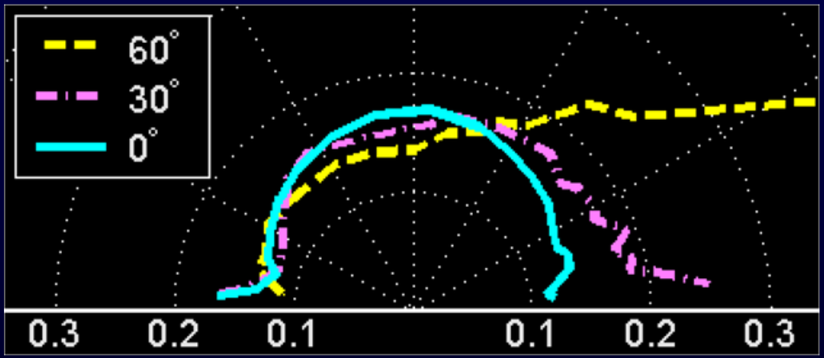
➢ Based on experimental observations of actual phenomena

- Characteristic spectral signatures
  - Example: effects of pigmentation on skin reflectance

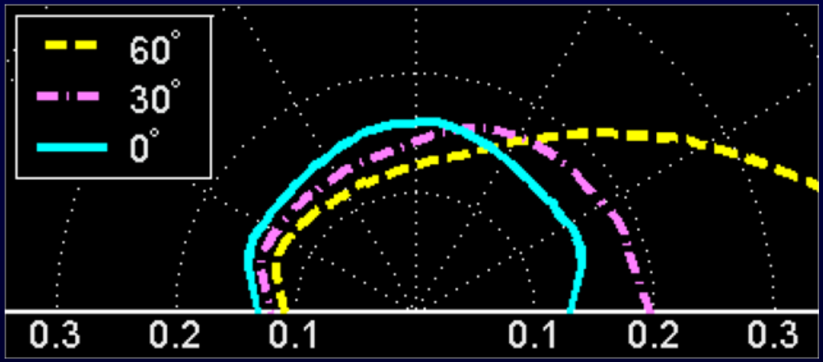


- Characteristic scattering profile
  - Example: angular dependence of skin specimens

Skin Scattering (BRDF) Data



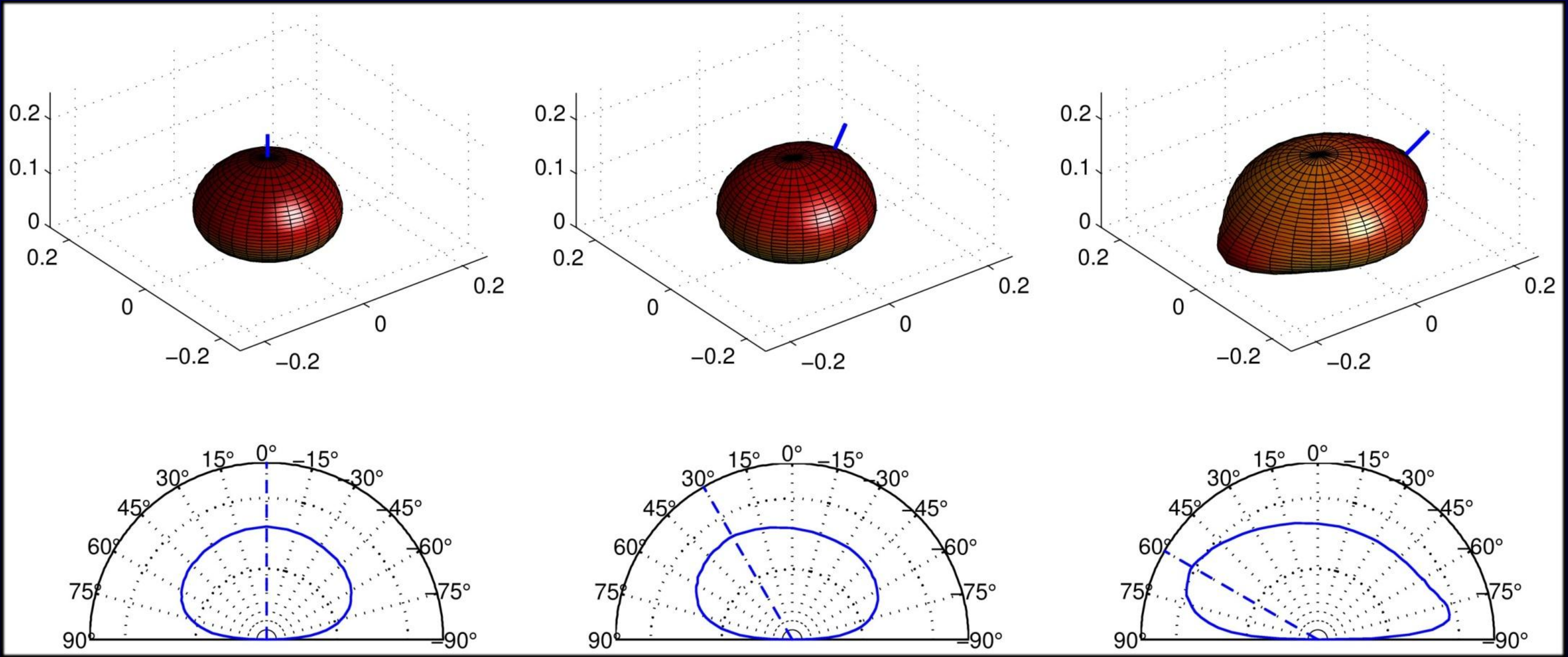
Cornell measured data



BioSpec modeled data

- Example: near Lambertian profile of sand samples, with some degree of forward scattering and retro-reflection for grazing angles

Simulated (SPLITS) BRDF Profiles



➢ Effectiveness of qualitative comparisons:

- They are less dependent on data availability issues

- They enable a broader assessment of the behavior of a model under different conditions

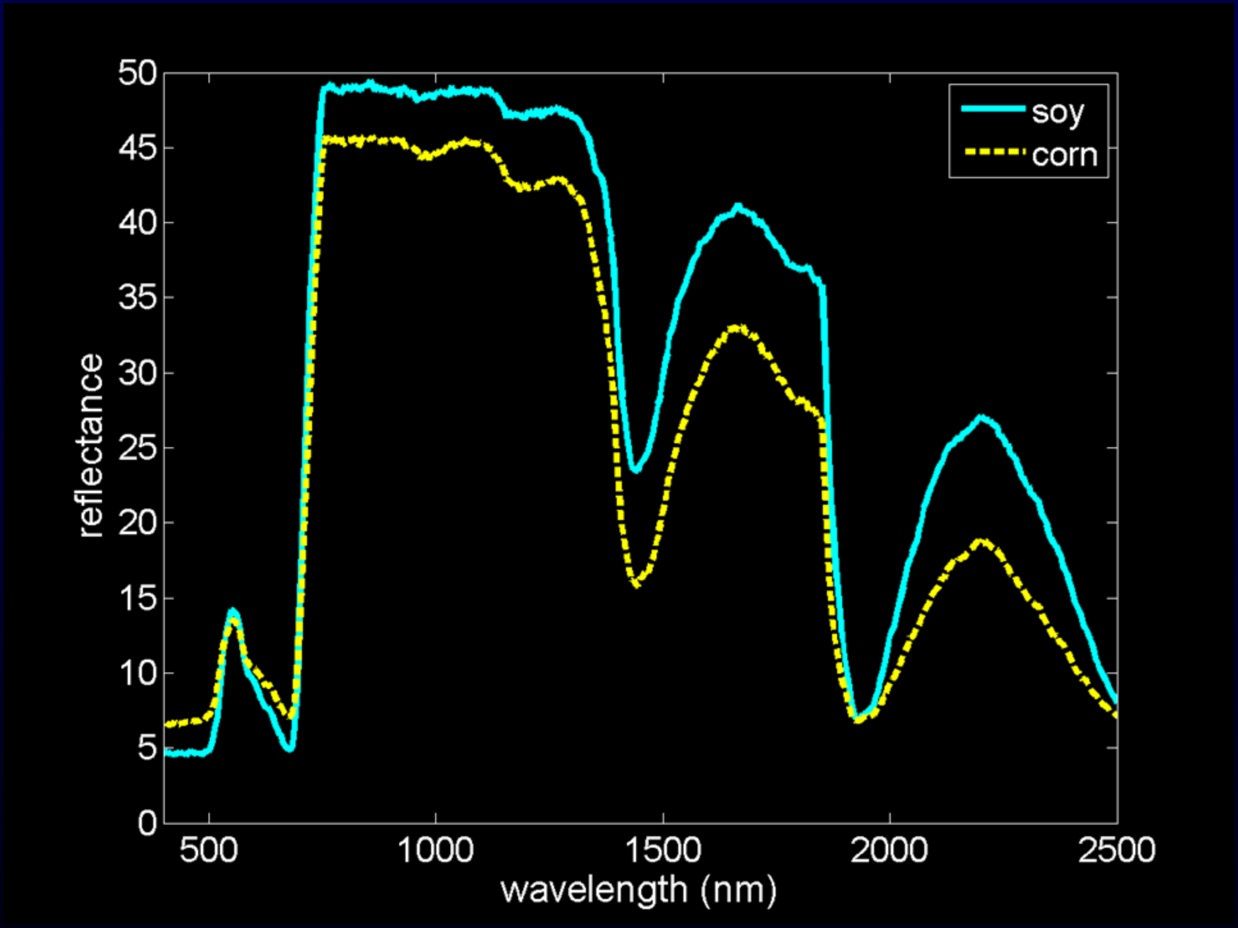
- They are less susceptible to experimental fluctuations

Newsprint

Cork

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

Typical Foliar Reflectance Curve

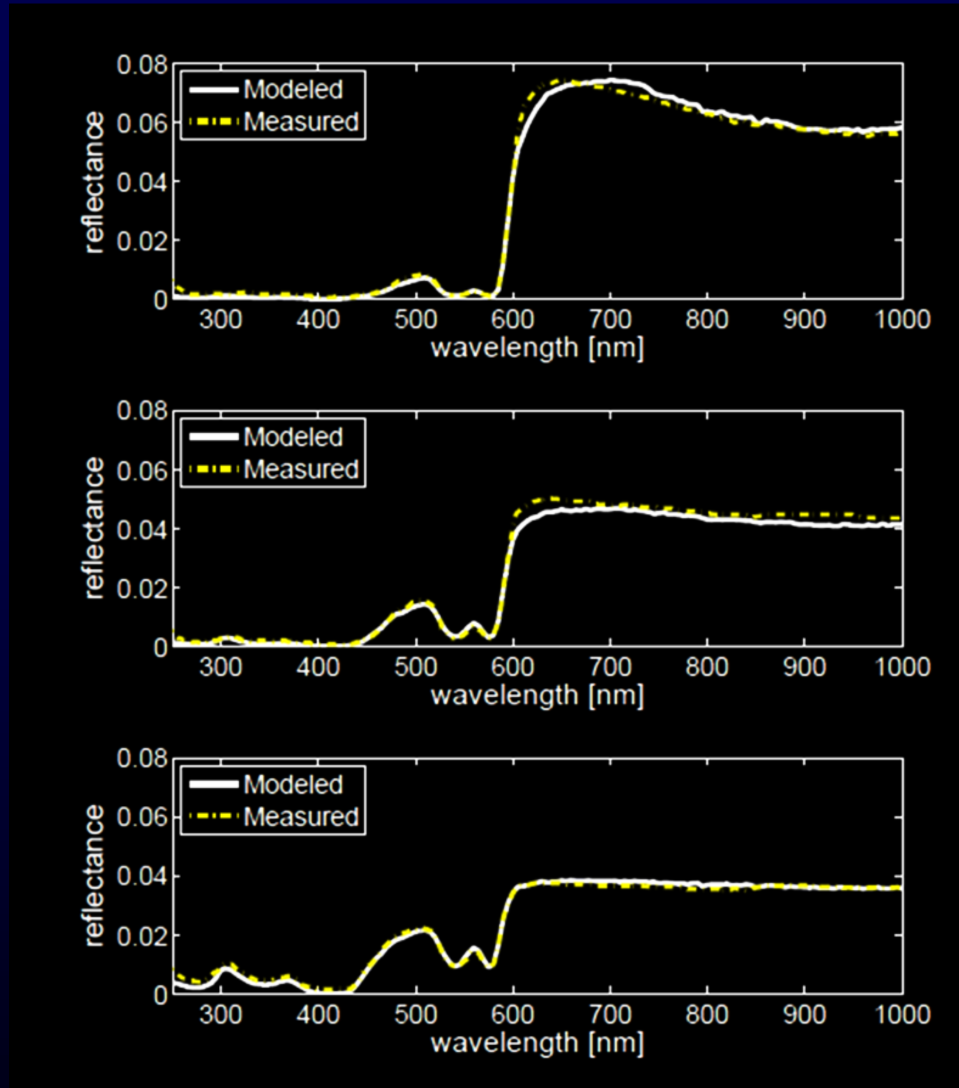


➢ General guidelines:

- In conjunction, quantitative and qualitative comparisons 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 *in silico* experiments

Example: Spectral Signatures of Blood Samples



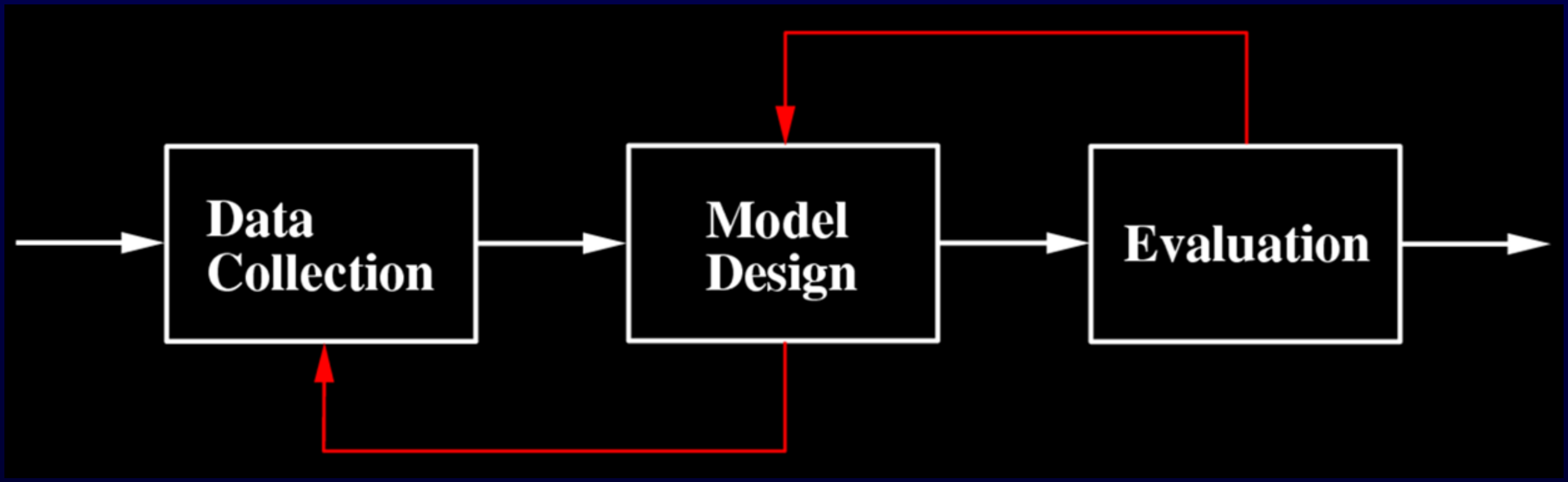
HCT = 0.33

HCT = 0.17

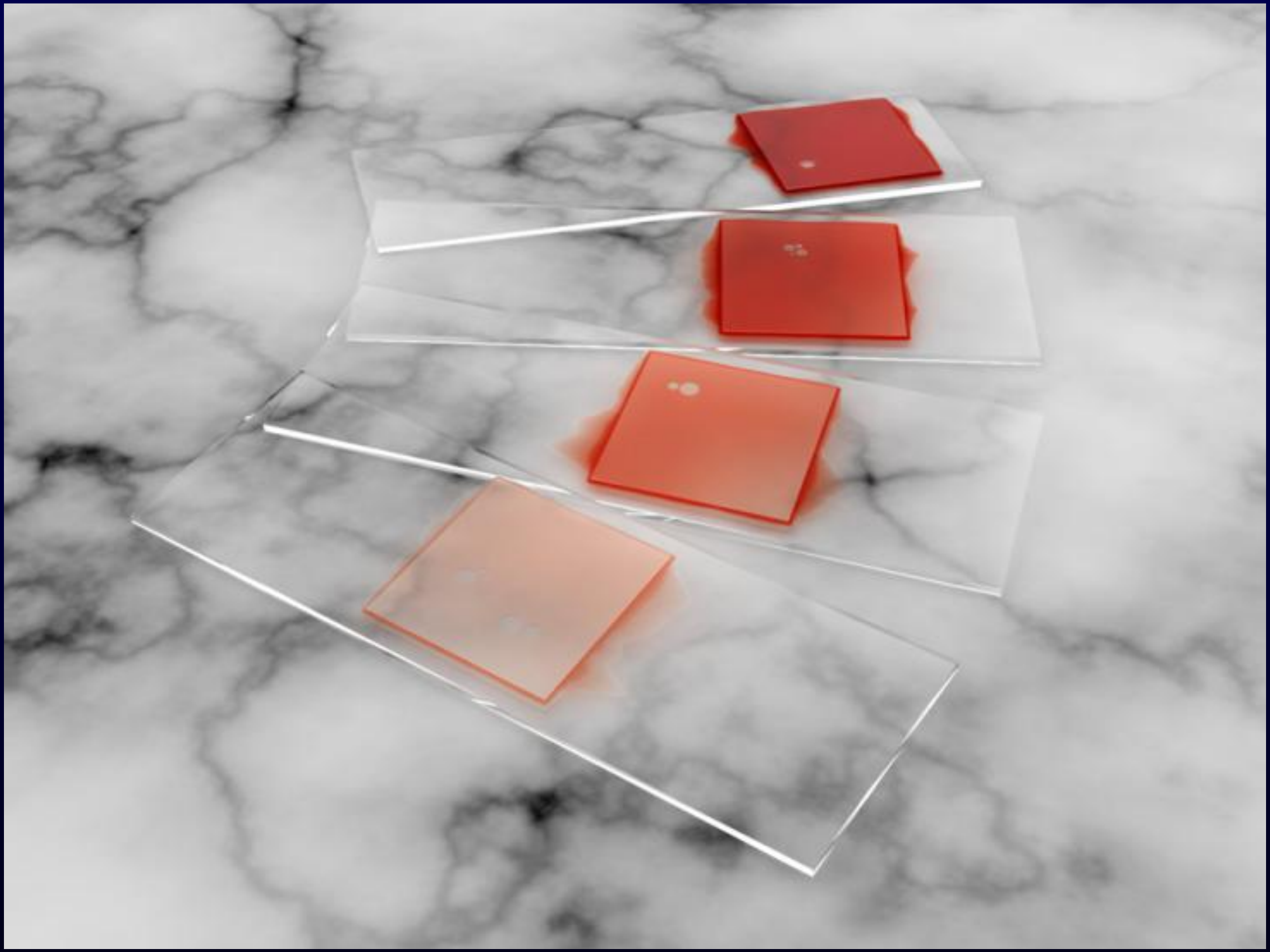
HCT = 0.084

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

- Recall the iterative nature the model development process



- Hence, a comprehensive evaluation approach pays off

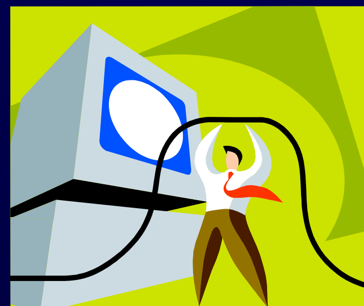


- In short, quantitative and qualitative comparisons with the “real thing”:
  - Rely on data availability
  - Complement each other
  - Facilitate the investigation of implementation errors
  - Enable the iterative refinement of the algorithms
  - Provide evidence of the fidelity of the simulations,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

Outline

- ✓ Parallel Comparisons
- ✓ Quantitative Comparisons
- ✓ Qualitative Comparisons
- ❑ Accuracy vs. Efficiency
- ❑ Reproducibility and Transparency

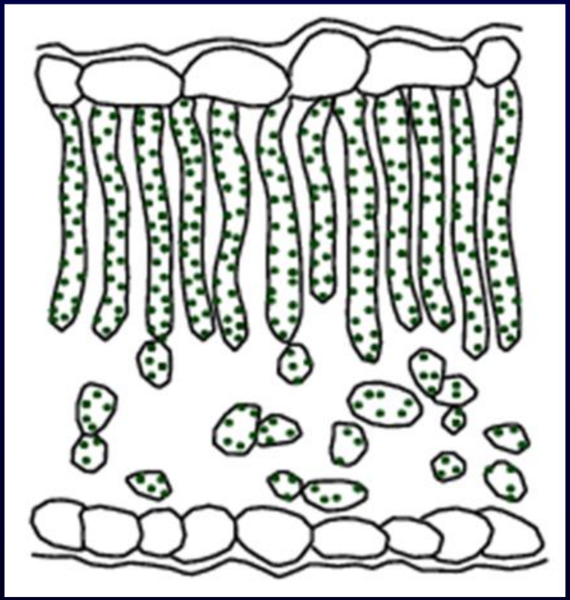
Accuracy vs. Efficiency



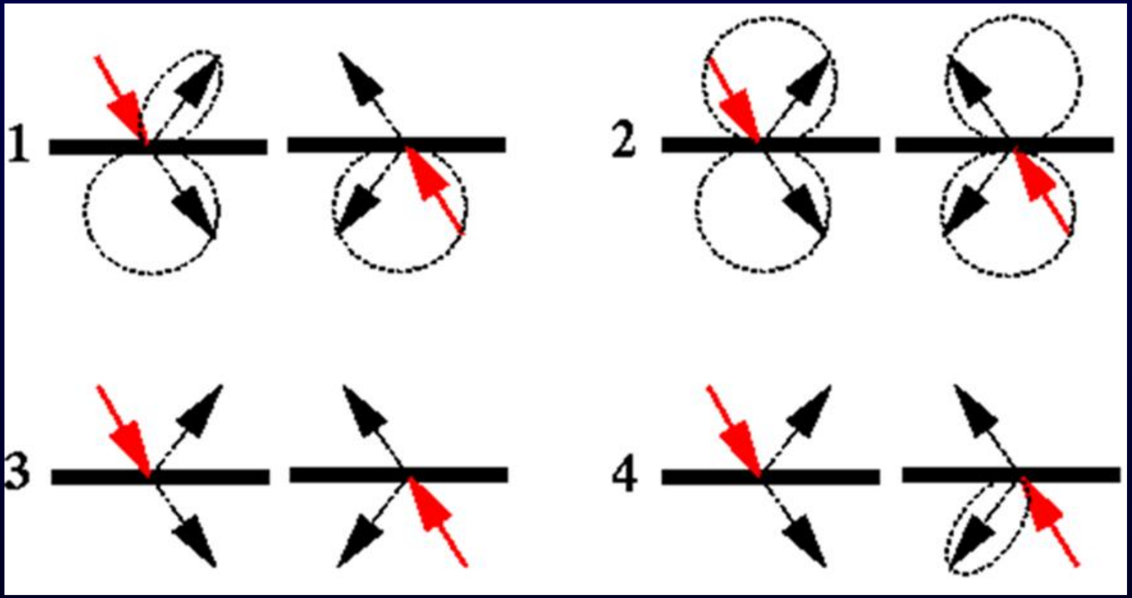
- Off-line schemes
  - Pre-computation strategies
  - Reconstruction techniques
    - ❖ Regression Analysis
    - ❖ Principal Component Analysis (PCA)
    - ❖ Piecewise Principal Component Analysis (PPCA)
    - ❖ Combination of PCA and regression analysis techniques

- Example of a pre-computation strategy:
  Recall the ABM model

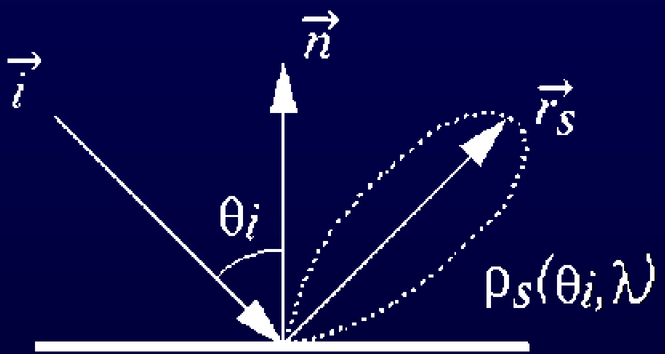
Cross-section



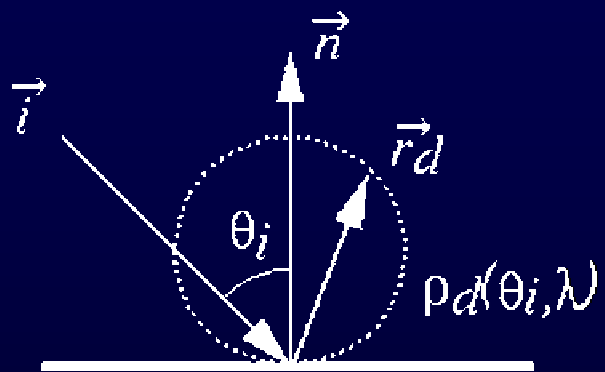
Layered ABM model for Plant Leaves



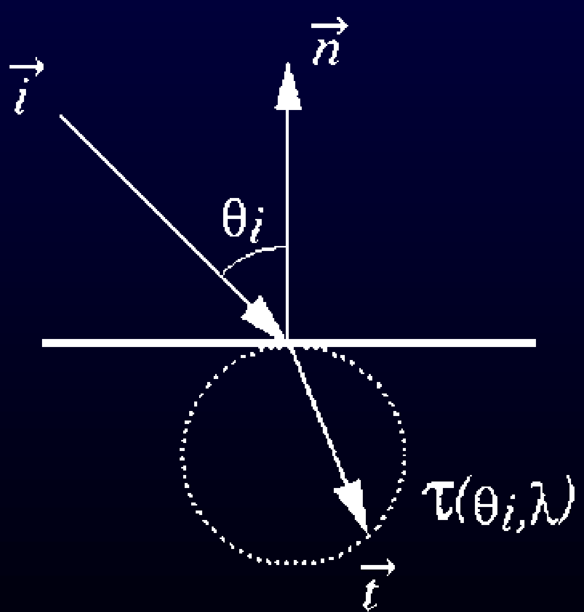
- Example of a pre-computation strategy:
  FSM (Foliar Scattering Model)



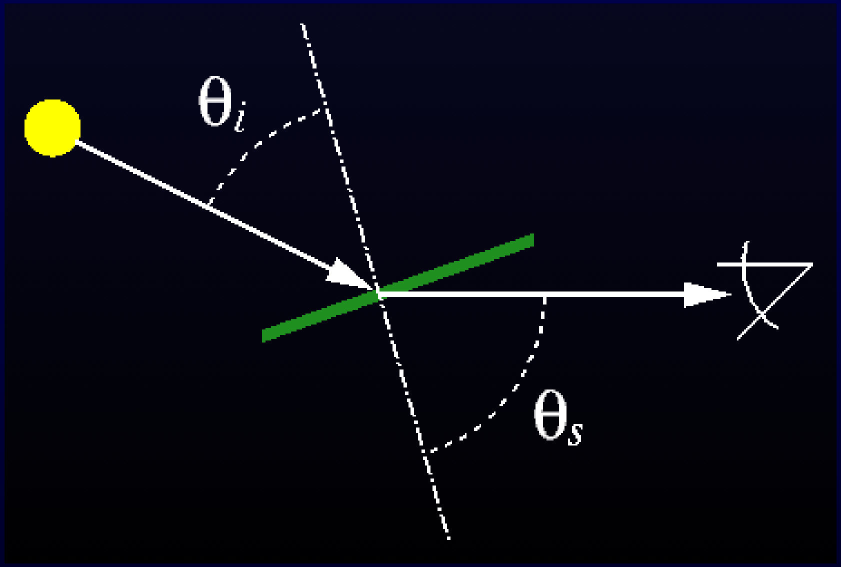
surface reflection



subsurface reflection



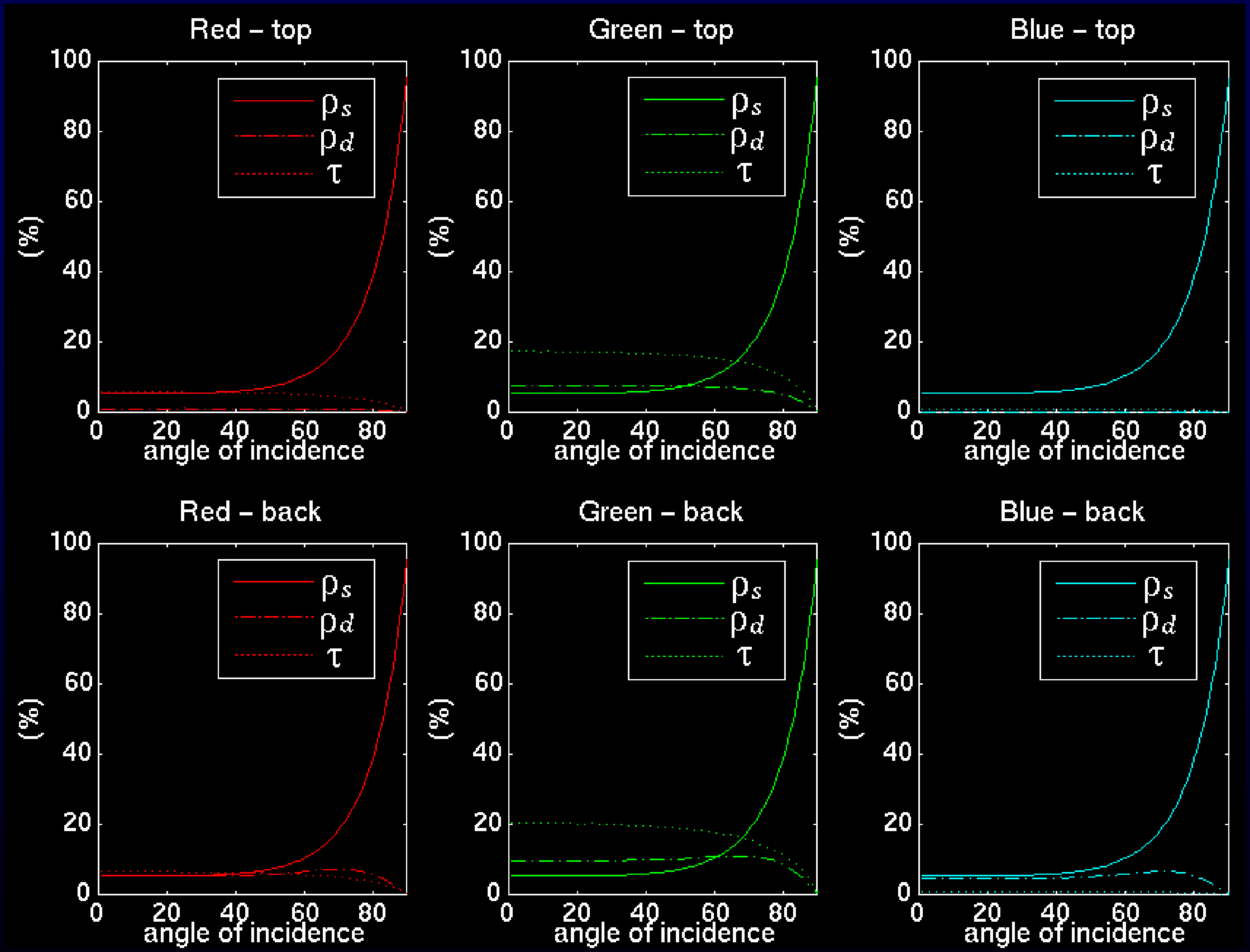
transmission


θi
θs

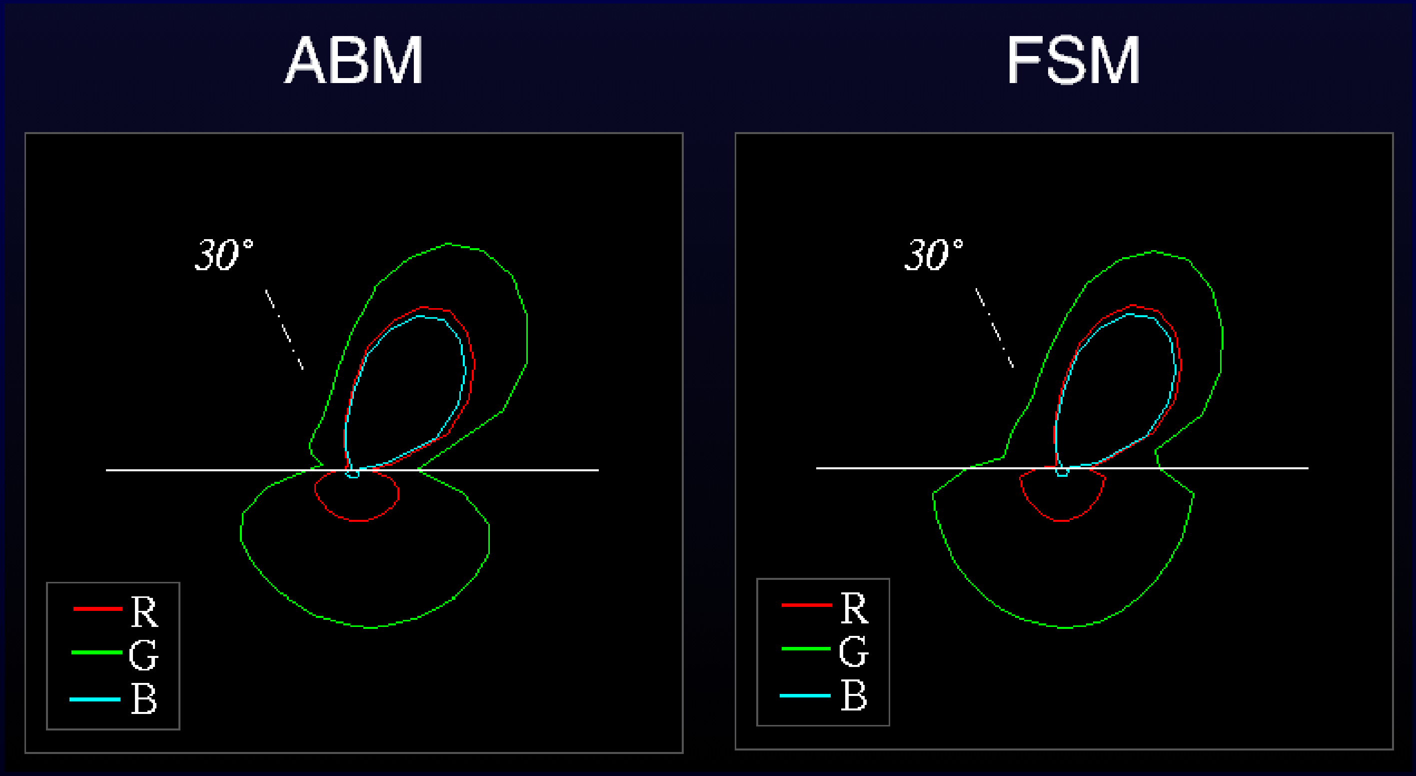
$$0^\circ < \theta_s \leq 90^\circ \quad \begin{cases} \dfrac{\rho_d(\theta_i, \lambda)}{\pi} & \text{if } 0^\circ < \theta_i \leq 90^\circ \\[2ex] \dfrac{\tau(\theta_i, \lambda)}{\pi} & \text{if } 90^\circ < \theta_i < 180^\circ \end{cases}$$

$$90^\circ < \theta_s < 180^\circ \quad \begin{cases} \dfrac{\tau(\theta_i, \lambda)}{\pi} & \text{if } 0^\circ < \theta_i \leq 90^\circ \\[2ex] \dfrac{\rho_d(\theta_i, \lambda)}{\pi} & \text{if } 90^\circ < \theta_i < 180^\circ \end{cases}$$

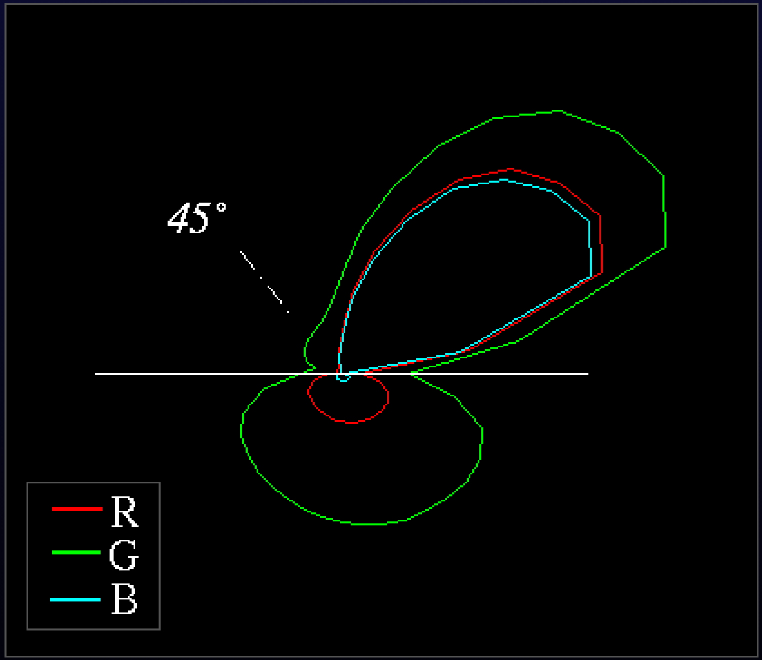
Spectral Curves Computed Using the ABM Model



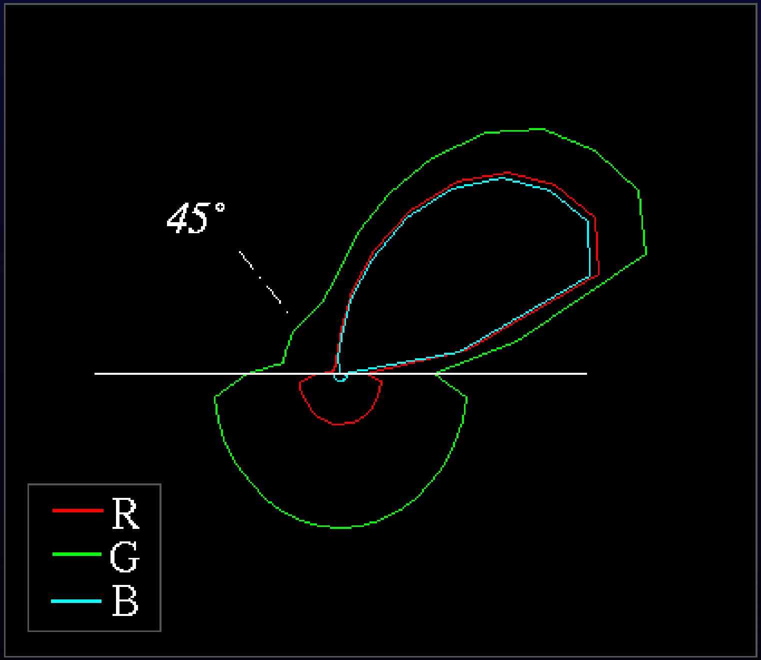
Comparison of BRDF and BTDF Spectral Curves



ABM



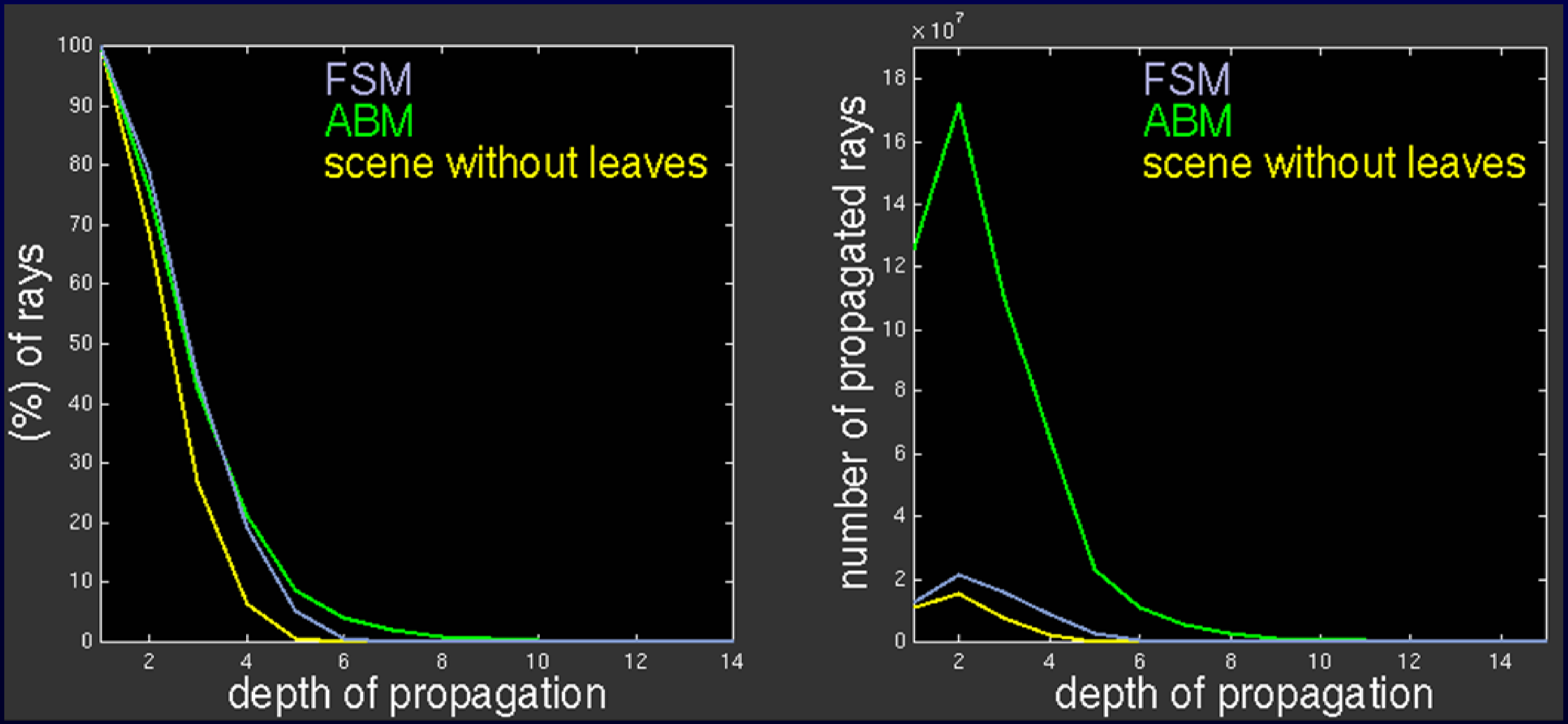
FSM



ABM

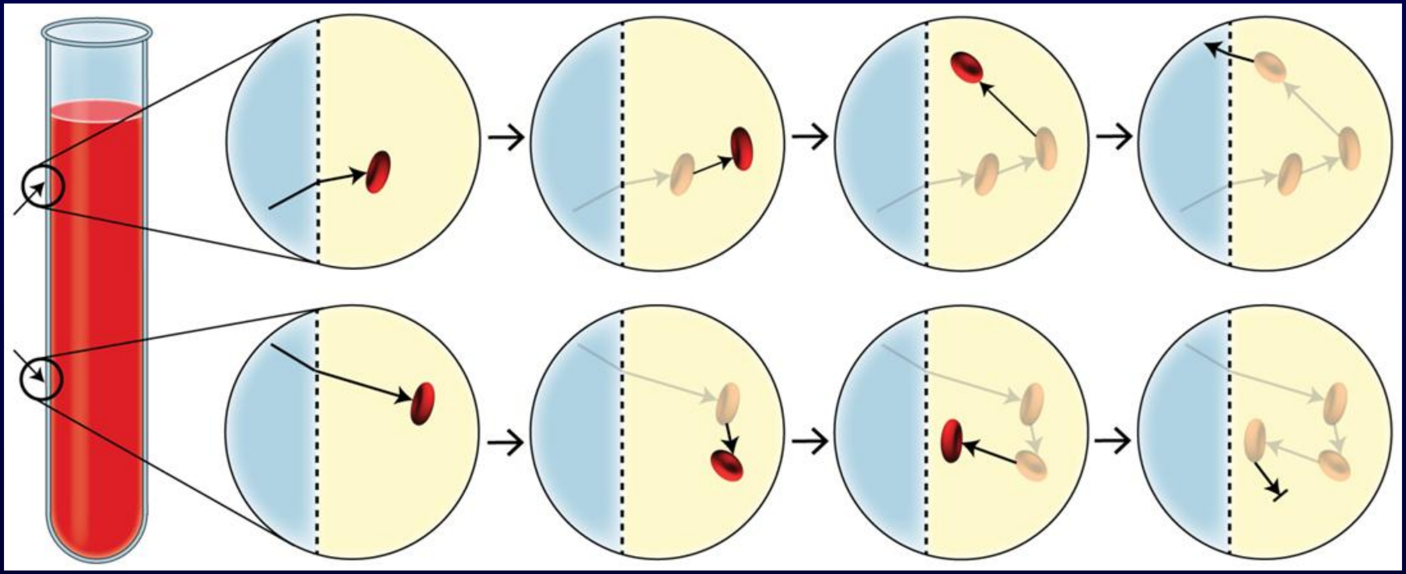
FSM

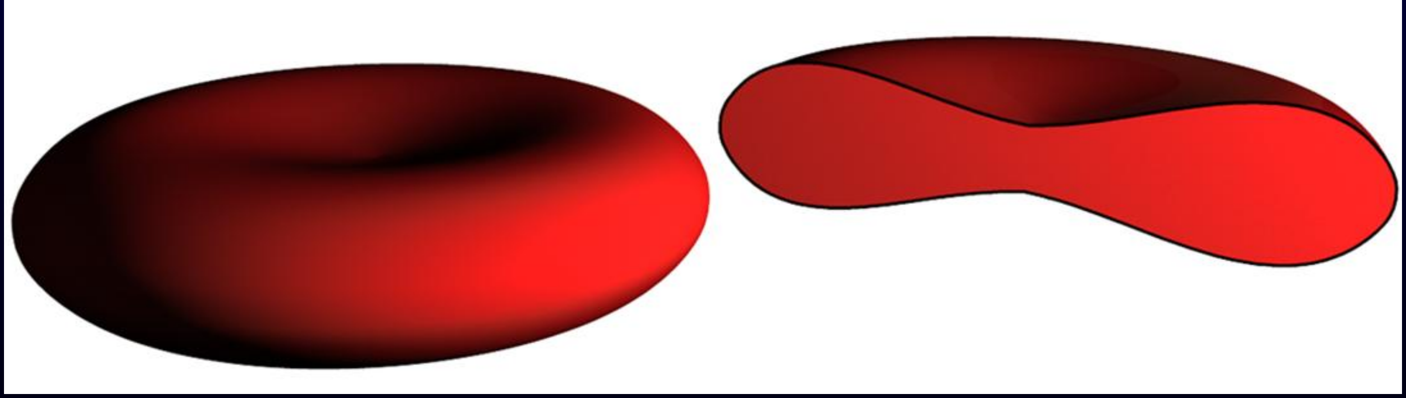
foliar ratio	RMS error			Speed-up
	R	G	B	
37.61%	0.020	0.016	0.012	9.77



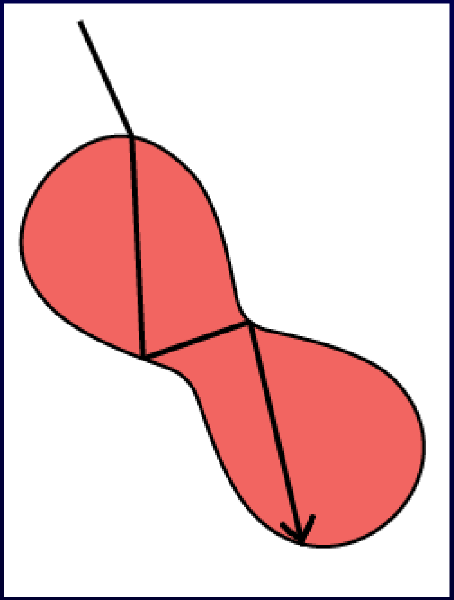
(%) of rays
FSM
ABM
scene without leaves
depth of propagation
x 10^7
number of propagated rays
FSM
ABM
scene without leaves
depth of propagation

- More “dramatic” example of a pre-computation strategy: Recall the CLBlood model





- Another example of a pre-computation strategy:
  Recall the CLBlood model

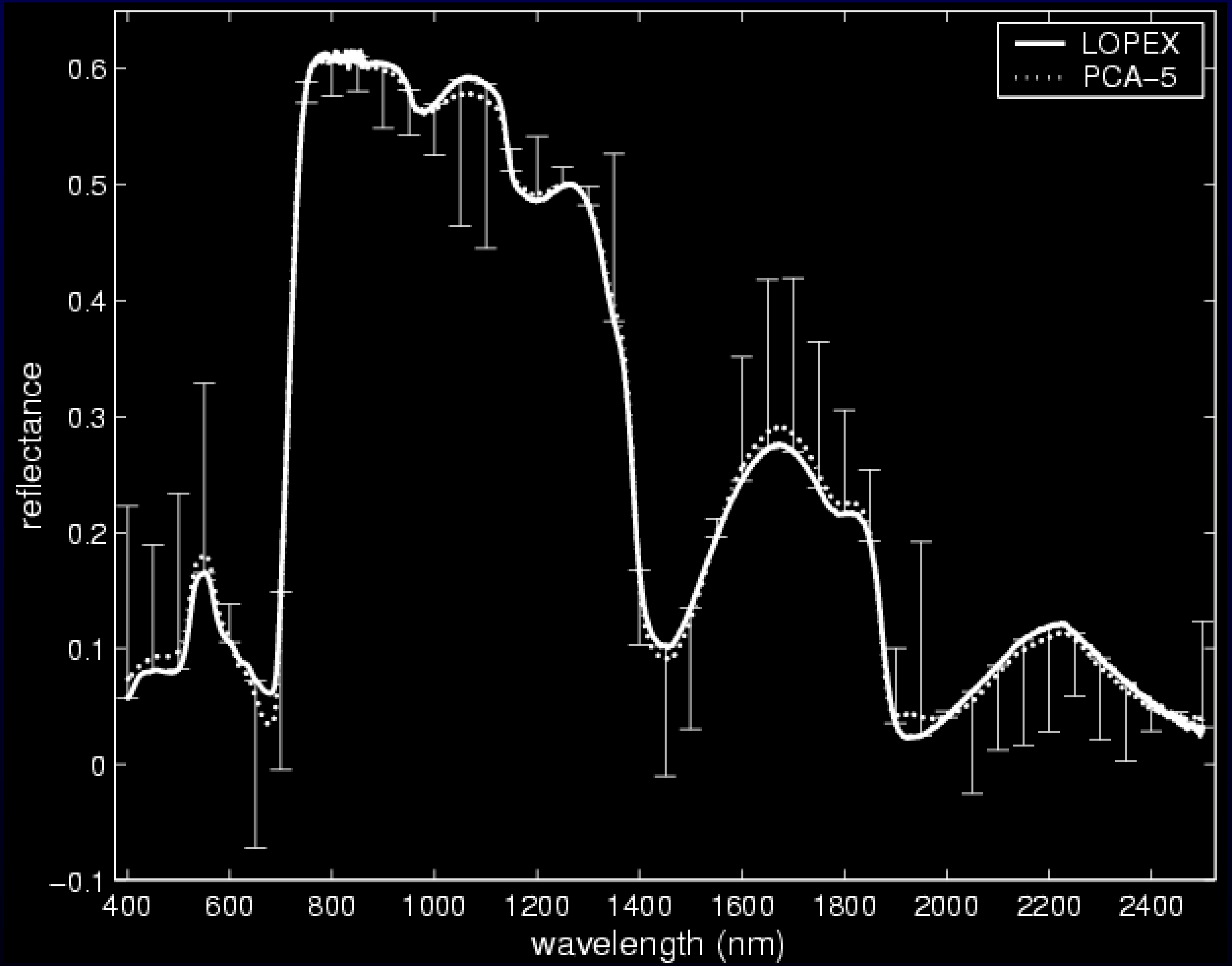


❖ cell reflection and absorption probabilities are pre-computed and stored considering different points and angles of incidence

❖ these values are accessed via table look-up during the simulations

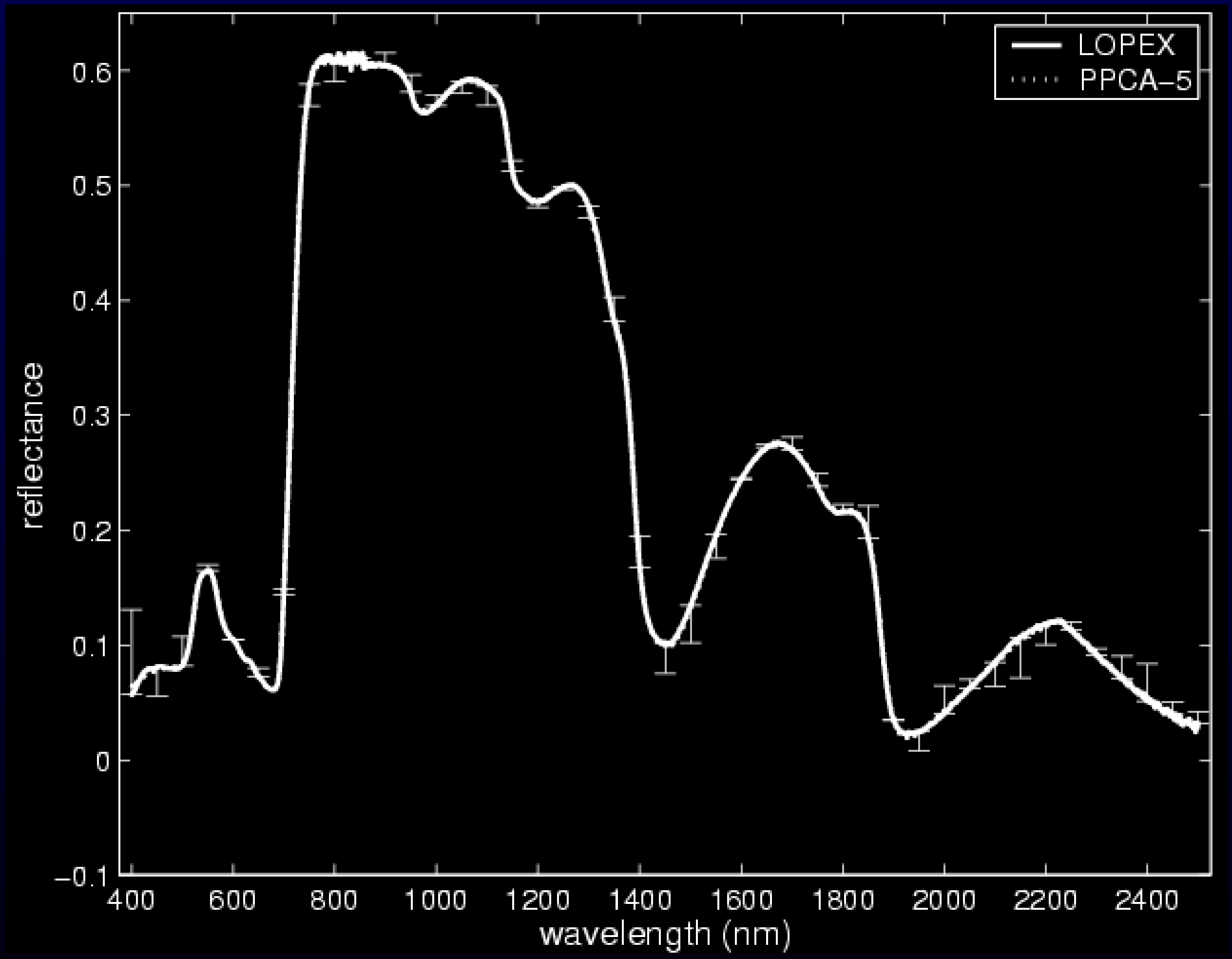
- Examples of reconstruction techniques

Foliar (Iris) Measured (LOPEX) and Reconstructed (PCA) Curves

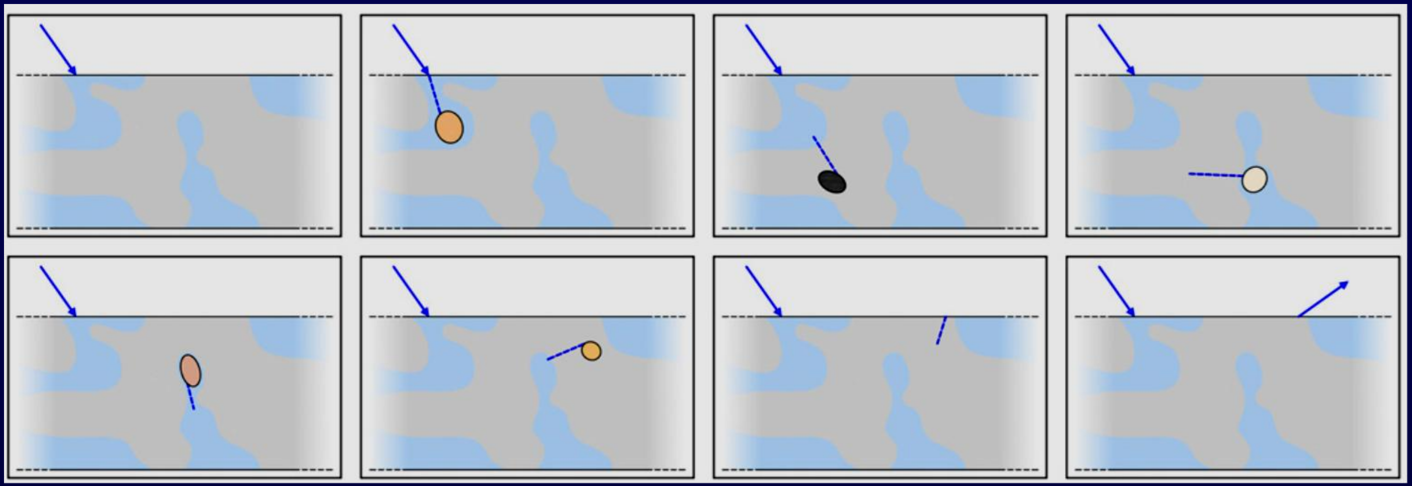


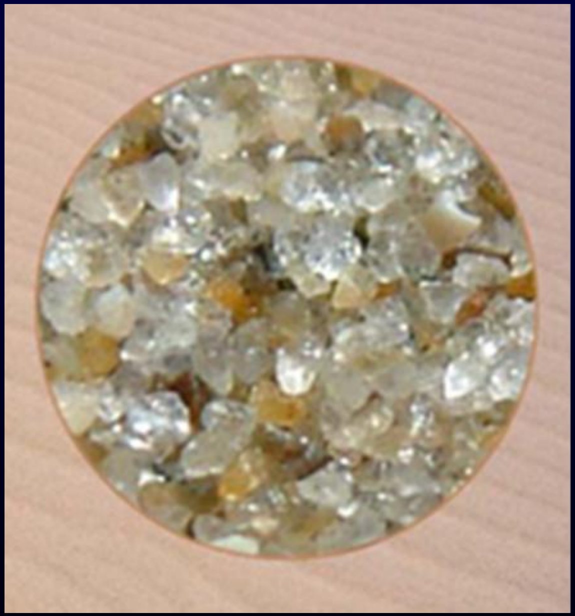
- Examples of reconstruction techniques

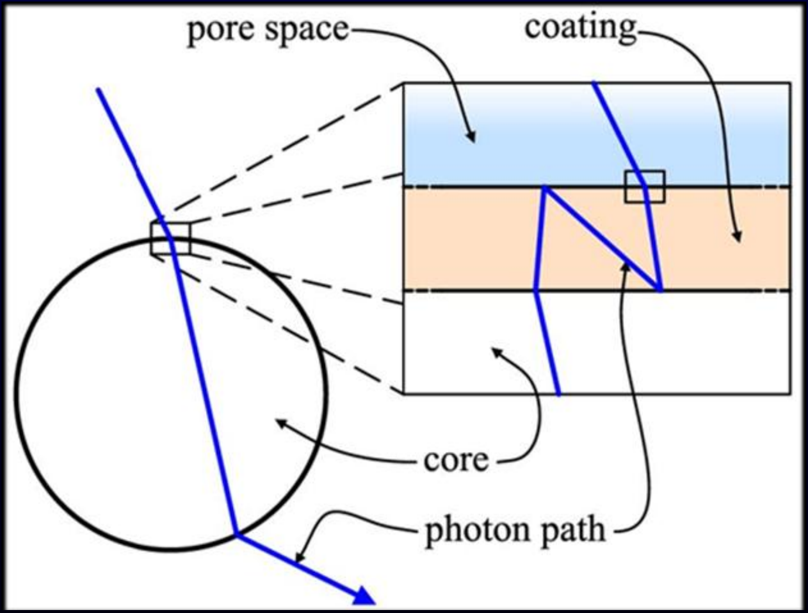
Foliar (Iris) Measured (LOPEX) and
Reconstructed (PPCA) Curves



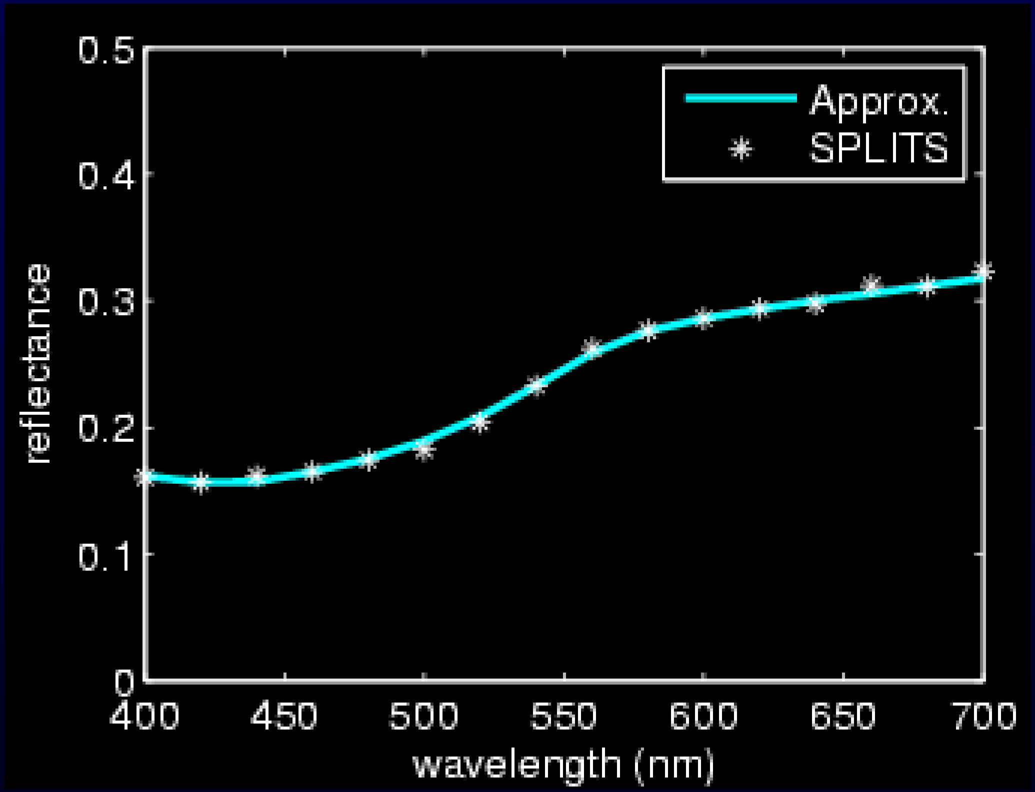
- Recall the SPLITS model



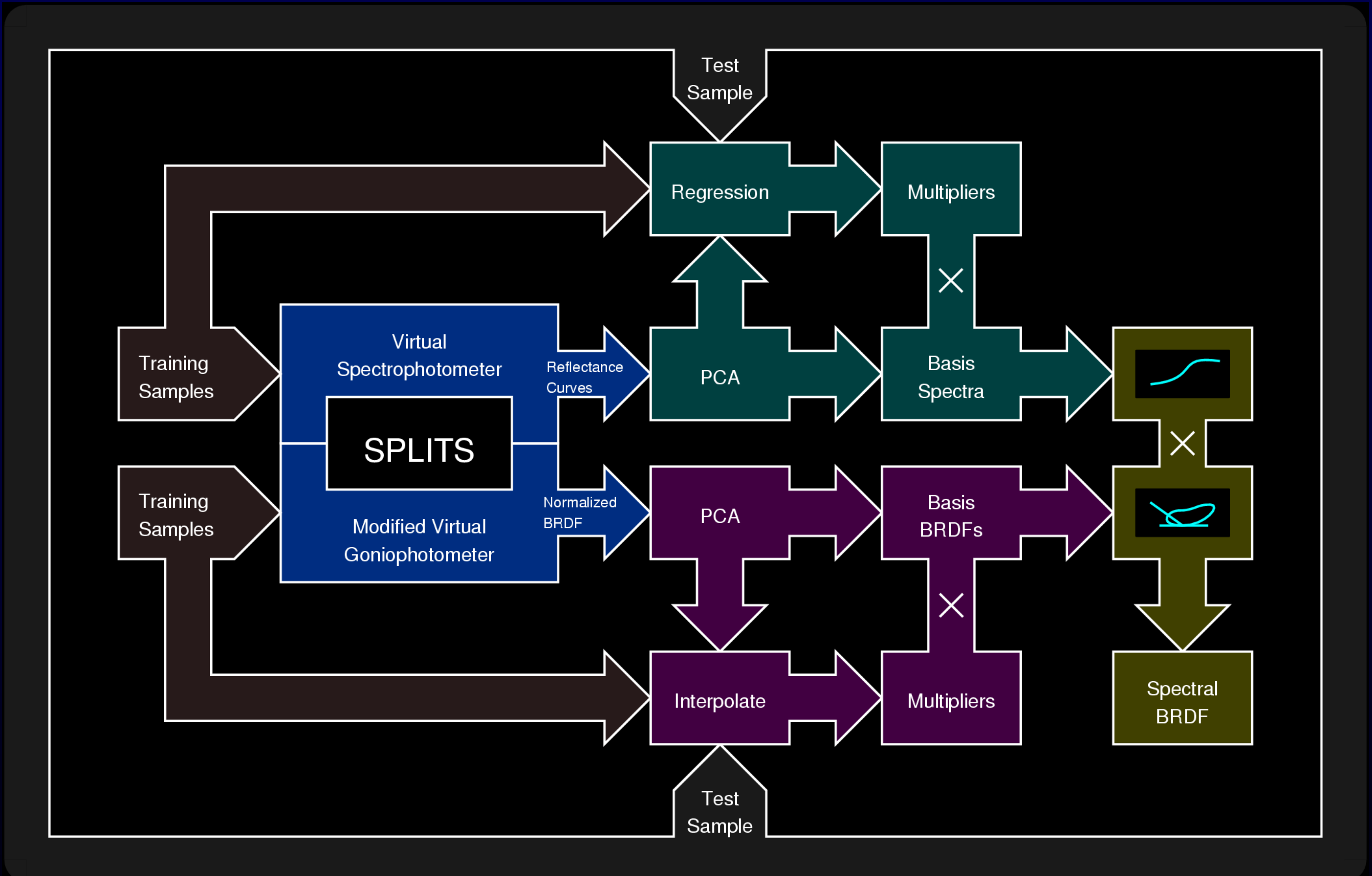


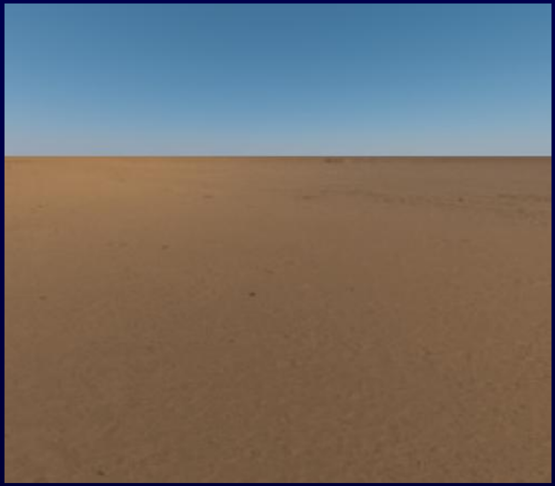


Sand Modeled (SPLITS) and Reconstructed (PCA + Regression) Curves



Combining PCA and Regression for Spectral BRDF Reconstruction





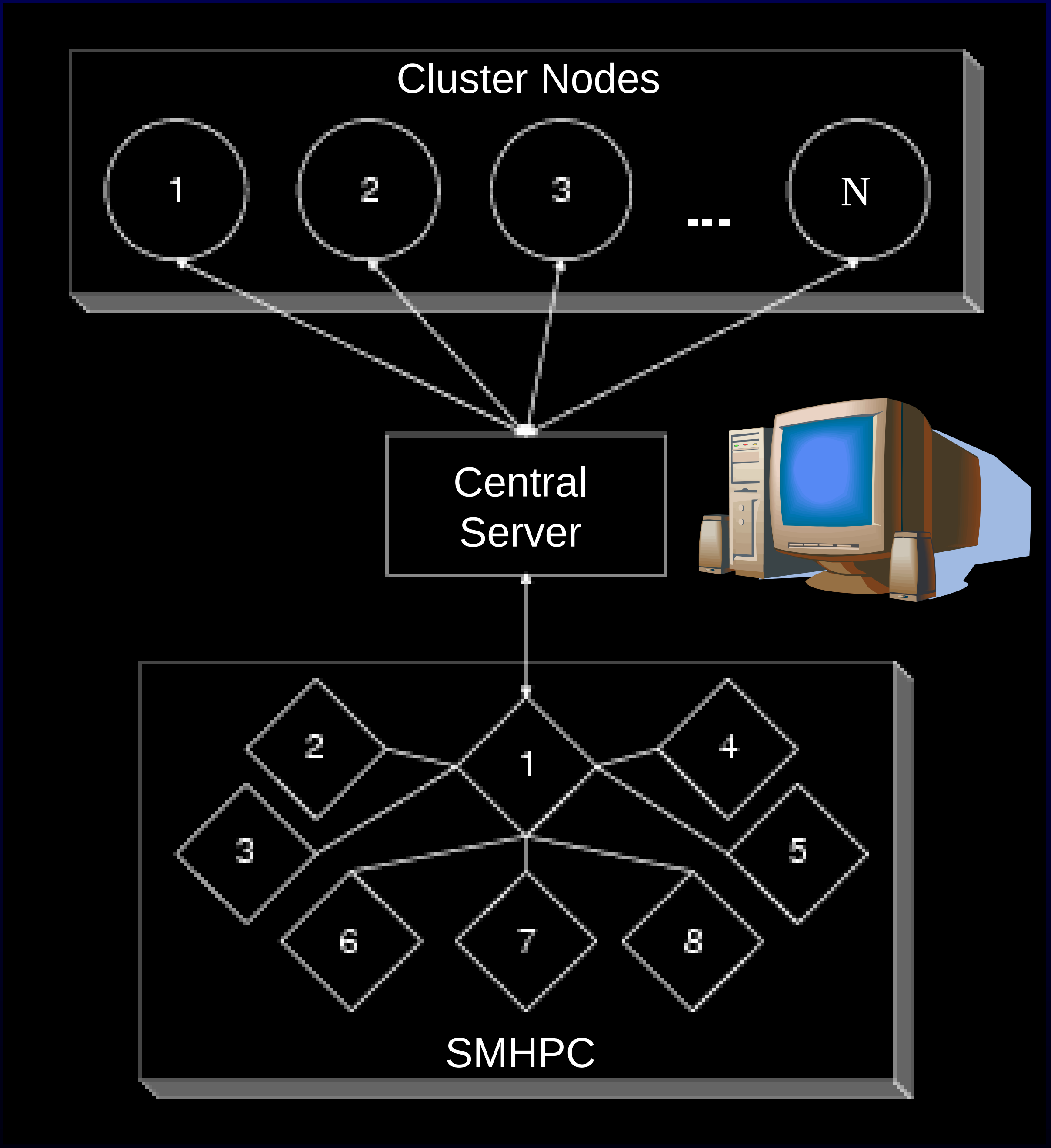
- Online schemes

  - Code optimization

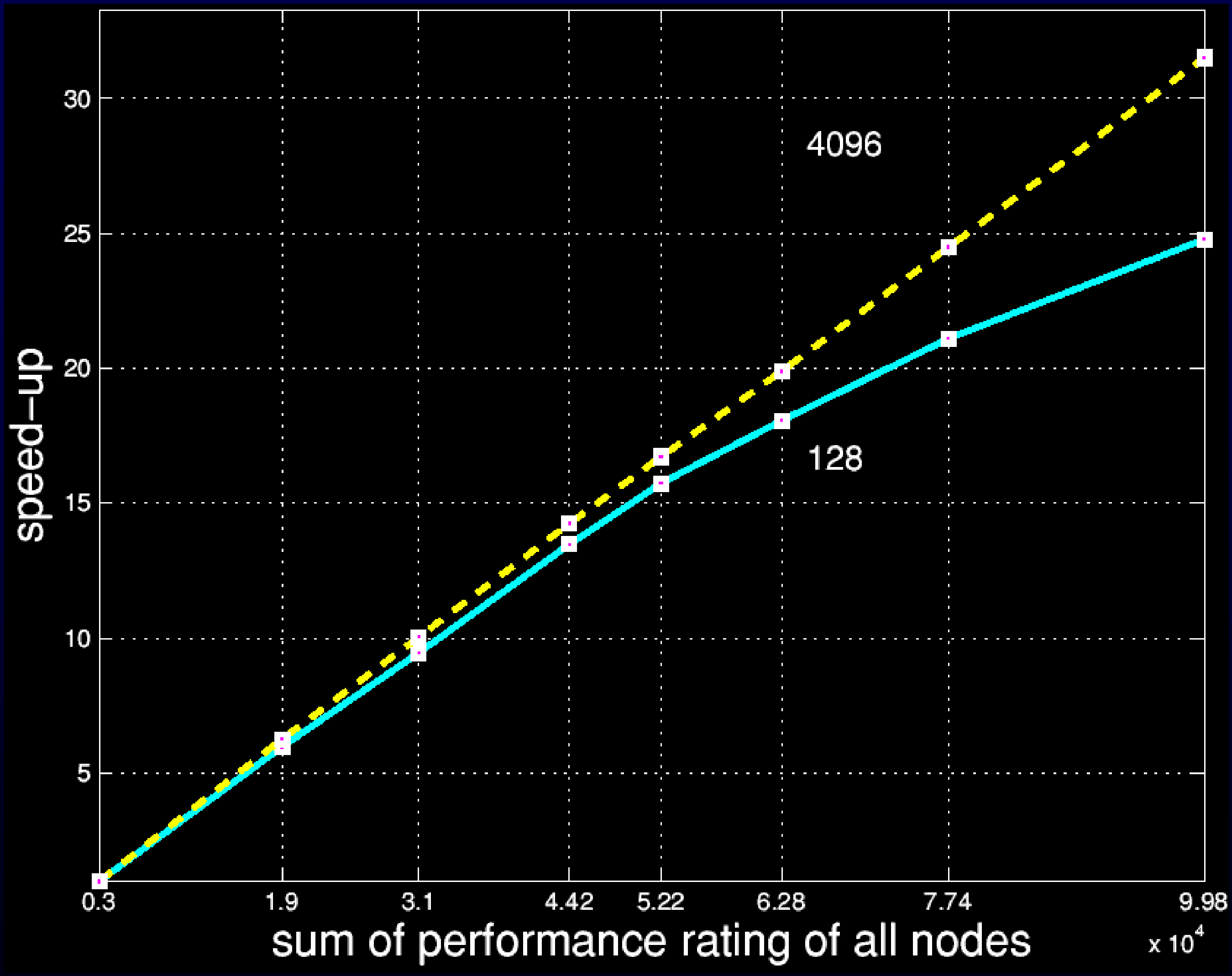
  - Parallel processing (software and hardware alternatives)

SMHPC

Cluster


Cluster Nodes
1
2
3
...
N
Central Server
1
2
3
4
5
6
7
8
SMHPC

Speed-ups for Two Sets of Simulations
(128 and 4096 samples)



- Specialized hardware

Graphics Processing Unit

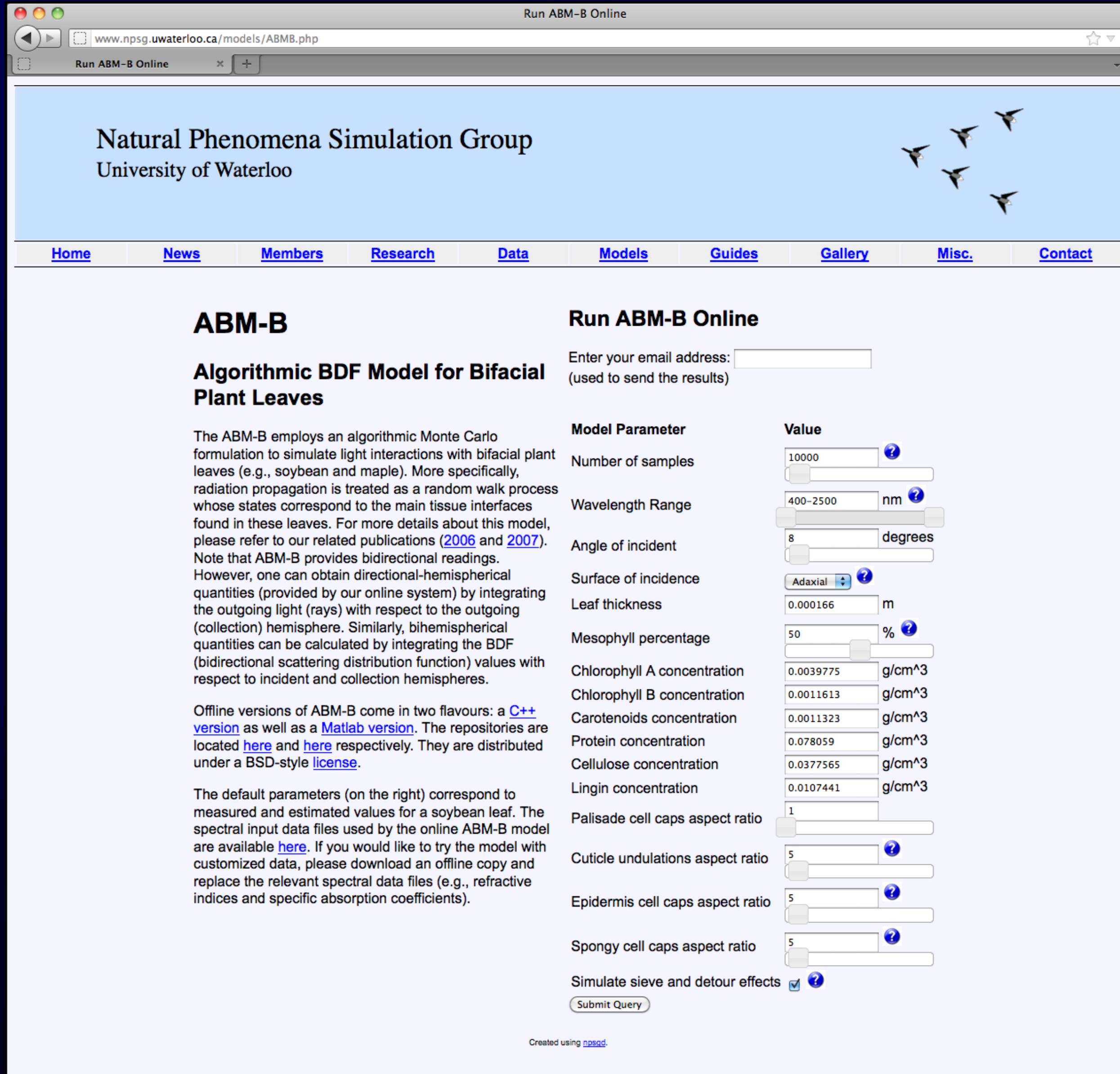
Outline

- ✓ Parallel Comparisons
- ✓ Quantitative Comparisons
- ✓ Qualitative Comparisons
- ✓ Accuracy vs. Efficiency
- ❑ Reproducibility and Transparency

Reproducibility and Transparency

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

- Code availability


Run ABM-B Online

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

Natural Phenomena Simulation Group
University of Waterloo

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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)

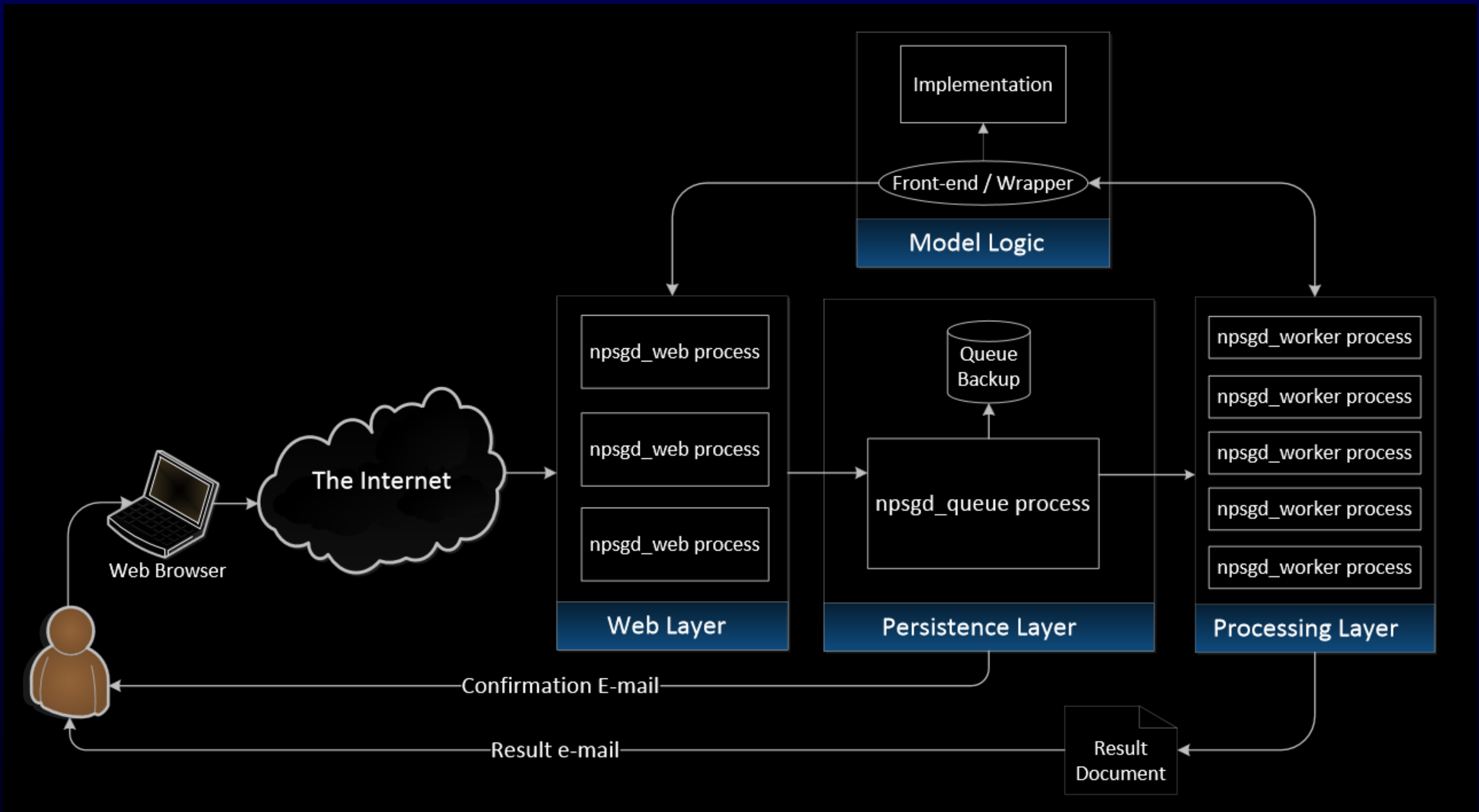
Model Parameter	Value
Number of samples	10000
Wavelength Range	400-2500 nm
Angle of incident	8 degrees
Surface of incidence	Adaxial
Leaf thickness	0.000166 m
Mesophyll percentage	50 %
Chlorophyll A concentration	0.0039775 g/cm^3
Chlorophyll B concentration	0.0011613 g/cm^3
Carotenoids concentration	0.0011323 g/cm^3
Protein concentration	0.078059 g/cm^3
Cellulose concentration	0.0377565 g/cm^3
Lingin concentration	0.0107441 g/cm^3
Palisade cell caps aspect ratio	1
Cuticle undulations aspect ratio	5
Epidermis cell caps aspect ratio	5
Spongy cell caps aspect ratio	5
Simulate sieve and detour effects	☑

Submit Query

Created using npsgd.

(IEEE Computer Graphics and Applications 2012)

Natural Phenomena Simulation Group Distributed - NPSGD



(IEEE Computer Graphics and Applications 2012)

"… 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?

- What are the “obstacles”?
  - “Fame” aspirations
  - Pressure to publish

- We should ask ourselves …

Do we want to be famous or useful?

- In summary, full dissemination of our work is essential for:
  - Overcoming reviewing “obstacles”
  - Getting the credit when it is deserved
  - Consolidating our contributions

This concludes Lecture 4!

Thanks!

Questions?

Credits: Images and Photos

- D. Yim
- M. Lam
- B. W. Kimmel
- A. Krishnaswamy
- T.F. Chen
- S.M. Hong
- T. Dimson
- Wikipedia