On-line Object Oriented Monte Carlo for the needs of Biophotonics and Biomedical Optics

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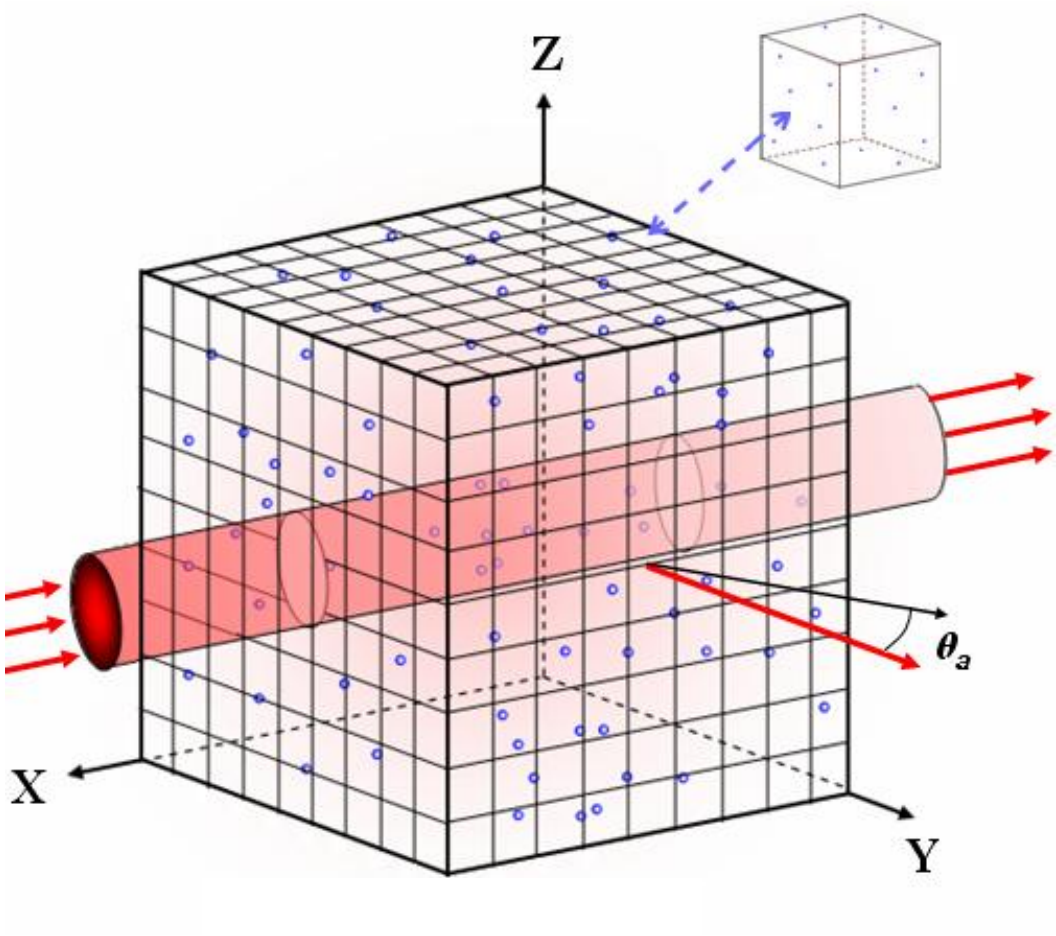
New Zealand
Cape Reinga
Bay of Islands
Whangerei
Hauraki Gulf
Auckland
Coromandel Peninsula
Tasman Sea
Bay of Plenty
Hamilton
Tauranga
North Island
Rotorua
Raukumara Range
Tongariro
National Park
Gisborne
Hawke Bay
Napier
Wanganui
Hastings
Tasman Bay
Abel Tasman
National Park
Nelson
Wellington
Westport
Blenheim
Cook Strait
Greymouth
Kaikura
South Island
Franz Josef Glacier
Fox Glacier
Pegasus Bay
Christchurch
Southern Alps
Map © bugbog.com
Milford Sound
Otago Peninsula
South Pacific Ocean
Dunedin
Invercargill
Stewart Island

Method Monte Carlo (MC)

- Started 1930 by Enrico Fermi (most famous early use) to the properties of the newly-discovered neutron.
- 1946 Stanislaw Ulam suggested to use random sampling to simulate path length of neutrons; 1947 developed by John von Newmann.
- 1949 Nick Metropolis and S. Ulam summarized the ideas.
- Since 1950s MC is actively used for work relating to the development of the nuclear/hydrogen bomb, atmospheric optics, geophysics, etc. (Meyer, Sobol, Marchuk; Abubakirov).
- 1980/90s: Noassal, Bonner, Chance, Feng, Kejzer, Prahl, Jacques, Wang, Yaroslavsky, Tuchin, Chernomordik and others are used MC for estimation of fluence rate distribution…
- Nowadays – 1000 papers in various optical diagnostic applications

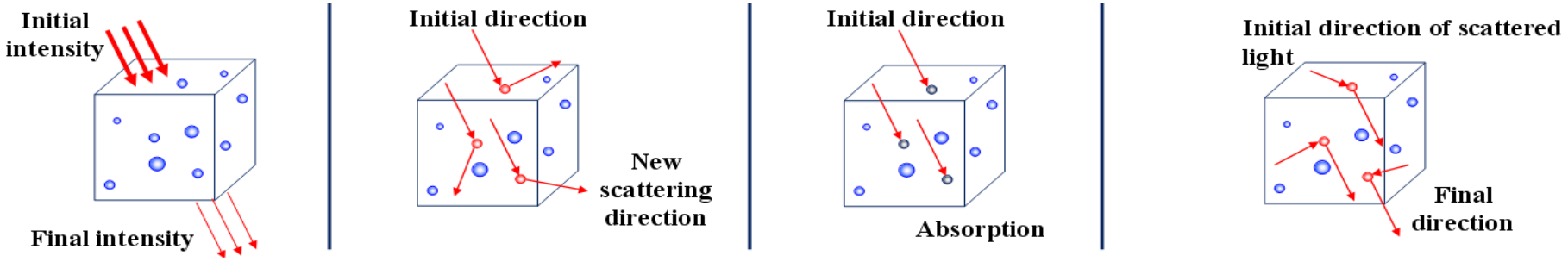
Scattering medium



Radiative Transfer

Radiative Transport Equation (RTE)

Change of light intensity in a volume V equals = Loss of intensity due to scattering in other directions (negative value) + Loss of intensity due to absorption (negative value) + Increase of the light intensity scattered from other directions into the initial direction (positive value)



$$\frac{1}{C}\frac{\partial I(\vec{r},\vec{s},t)}{\partial t} = -\mu_s I(\vec{r},\vec{s},t) - \mu_a I(\vec{r},\vec{s},t) + \mu_s \int_{4\pi} f(\vec{s}',\vec{s}) I(\vec{r},\vec{s},t) d\Omega'$$

Monte Carlo modeling

- **Optical Radiation is defined by photon packets (photons):**
  - → Photons propagate through the scattering medium with an initial parameters that are corresponding to the light source geometry/properties
- **Trajectory of each photon is governed by Probability Density Functions:**
  - → Probability to be absorbed along the path length l
  - → Probability to be scattered along the path length l
  - → Probability to change the direction depending on the scattering phase function ex: Rayleigh, Lorentz-Mie, Henyey-Greenstein, etc.
- **Detected photons are characterized by:**
  - → Number of scatter events
  - → Final photon position and direction
  - → Total path length and time of flight
- **Exact solution of RTE:**
  - → Infinite number of photons sent

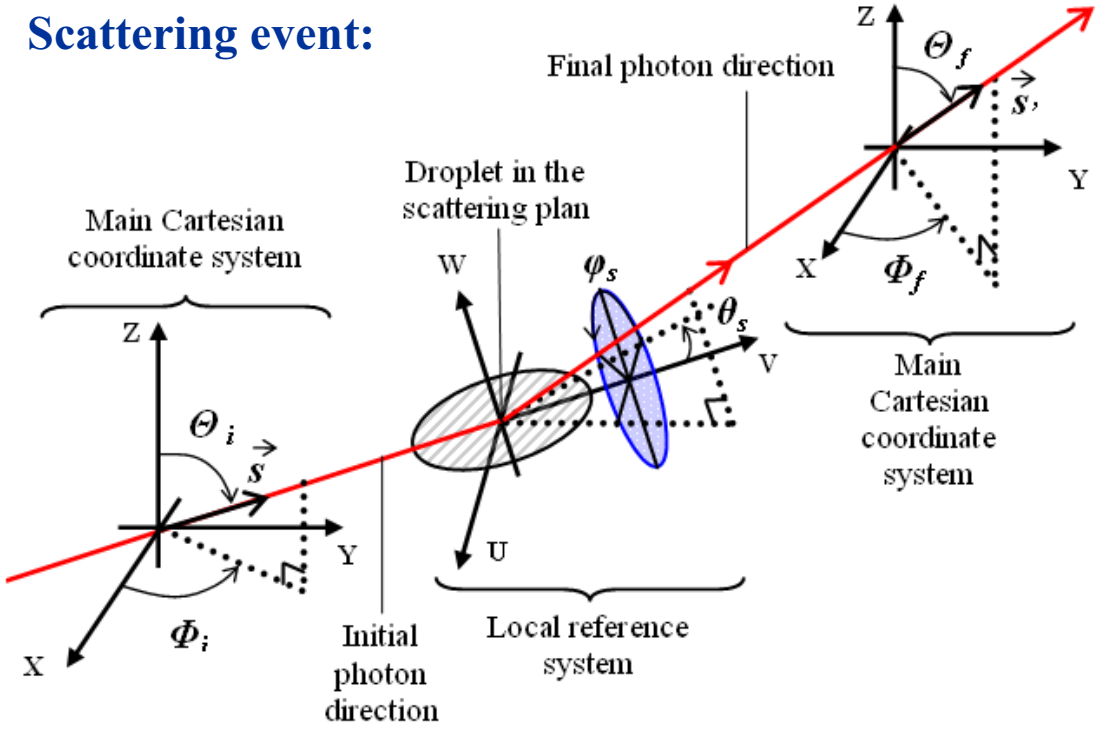
Monte Carlo modelling

Free path length at each scattering events:

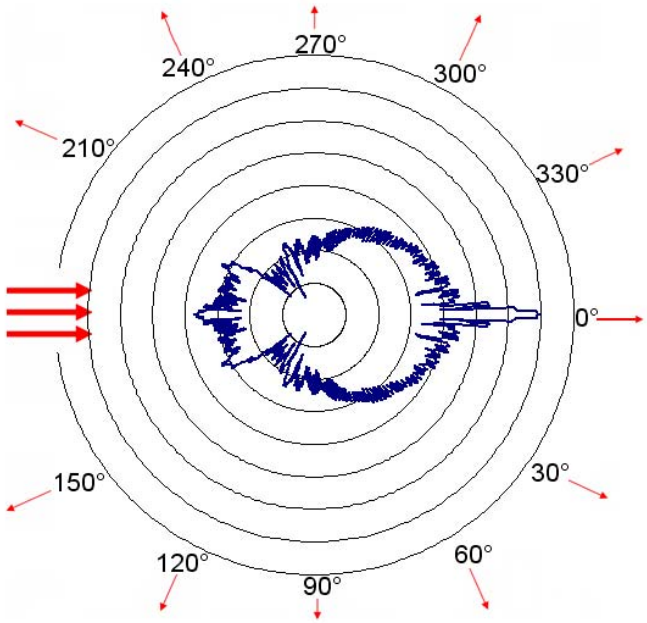
$$l_i = -\frac{\ln(\xi)}{\mu_e}$$

ξ : **Random Number**

Scattering event:

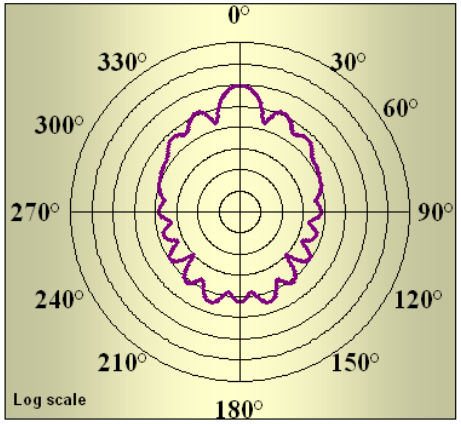


Example of a Lorentz-Mie scattering phase function $f(\theta s)$:



Monte Carlo modeling

Scattering phase function:



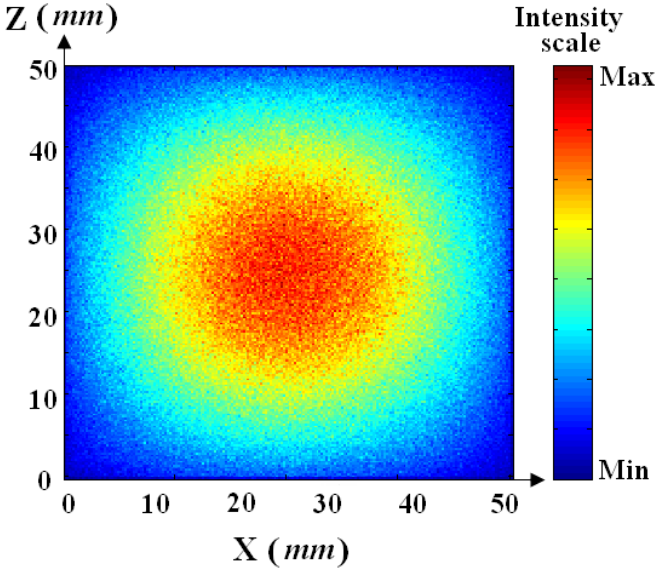
Diameter: 1.0 μ m

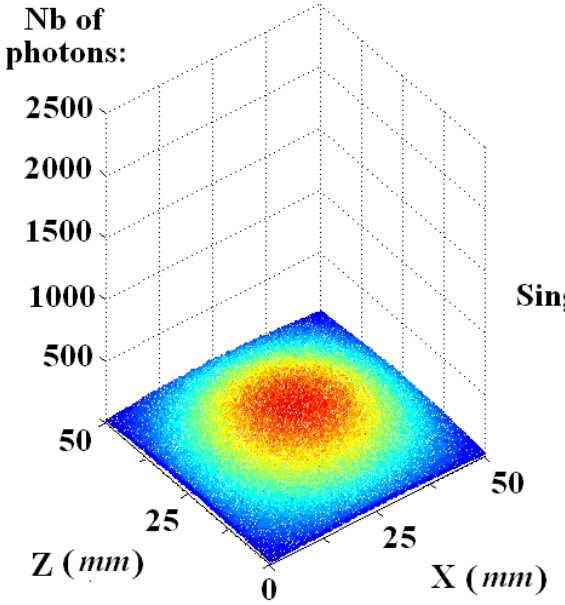
Front face

Single + Multiple scattering

$\theta_a = 90^\circ$

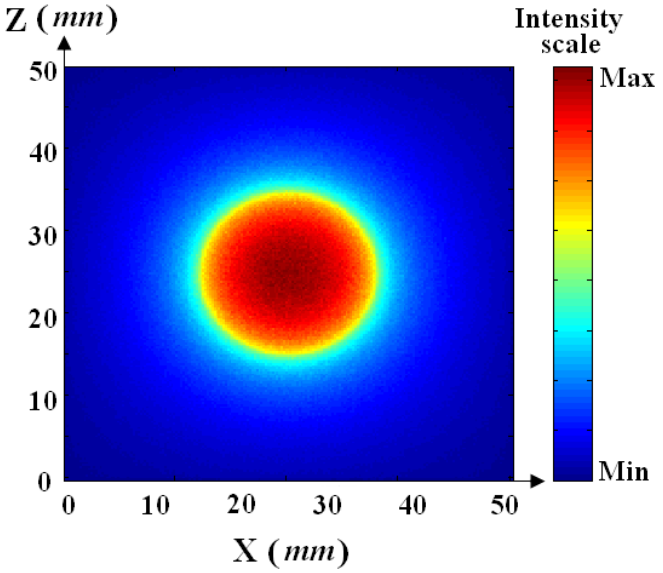
$\mu_{sca} = 0.24\ mm^{-1}$



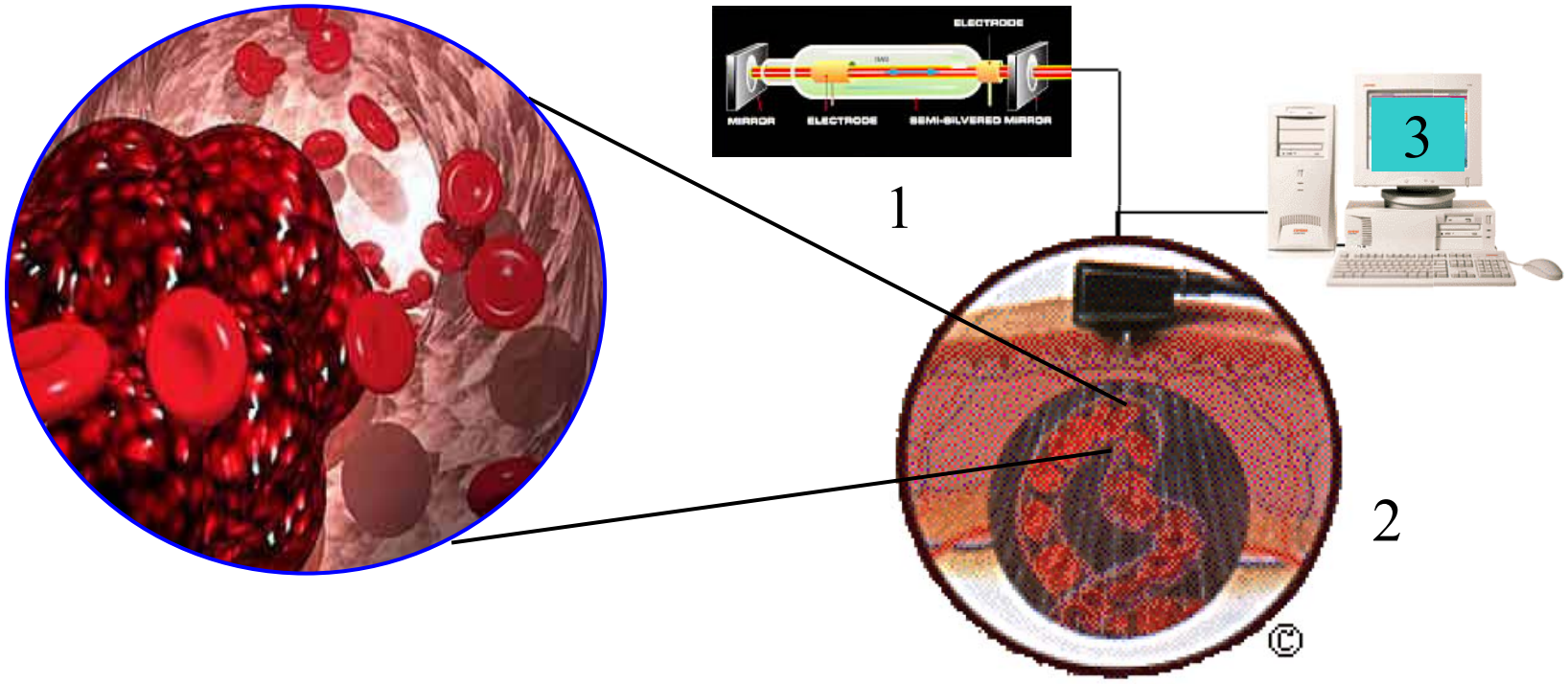


Back face

Single + Multiple scattering

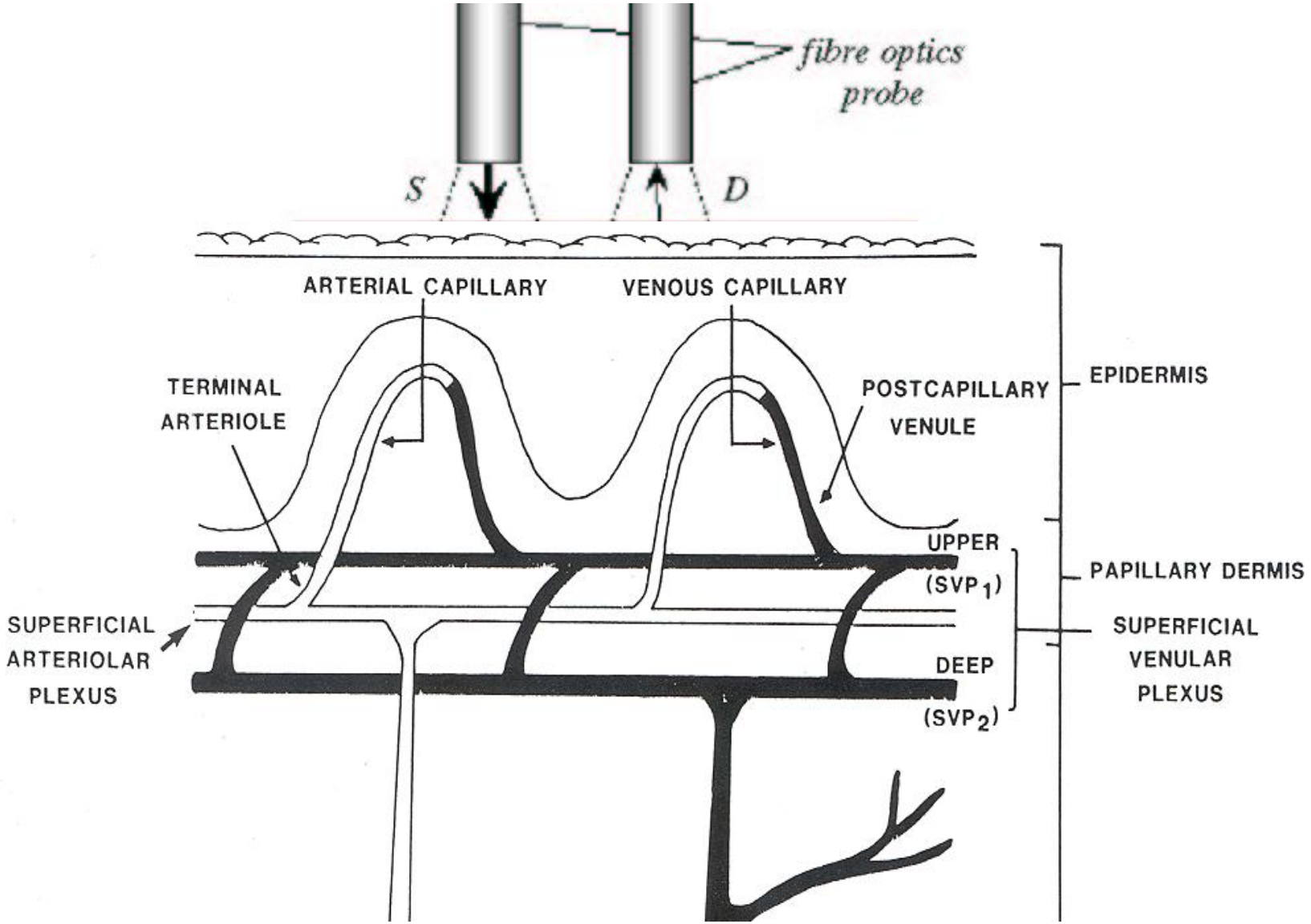


Typical Optical Diagnostic Experiment

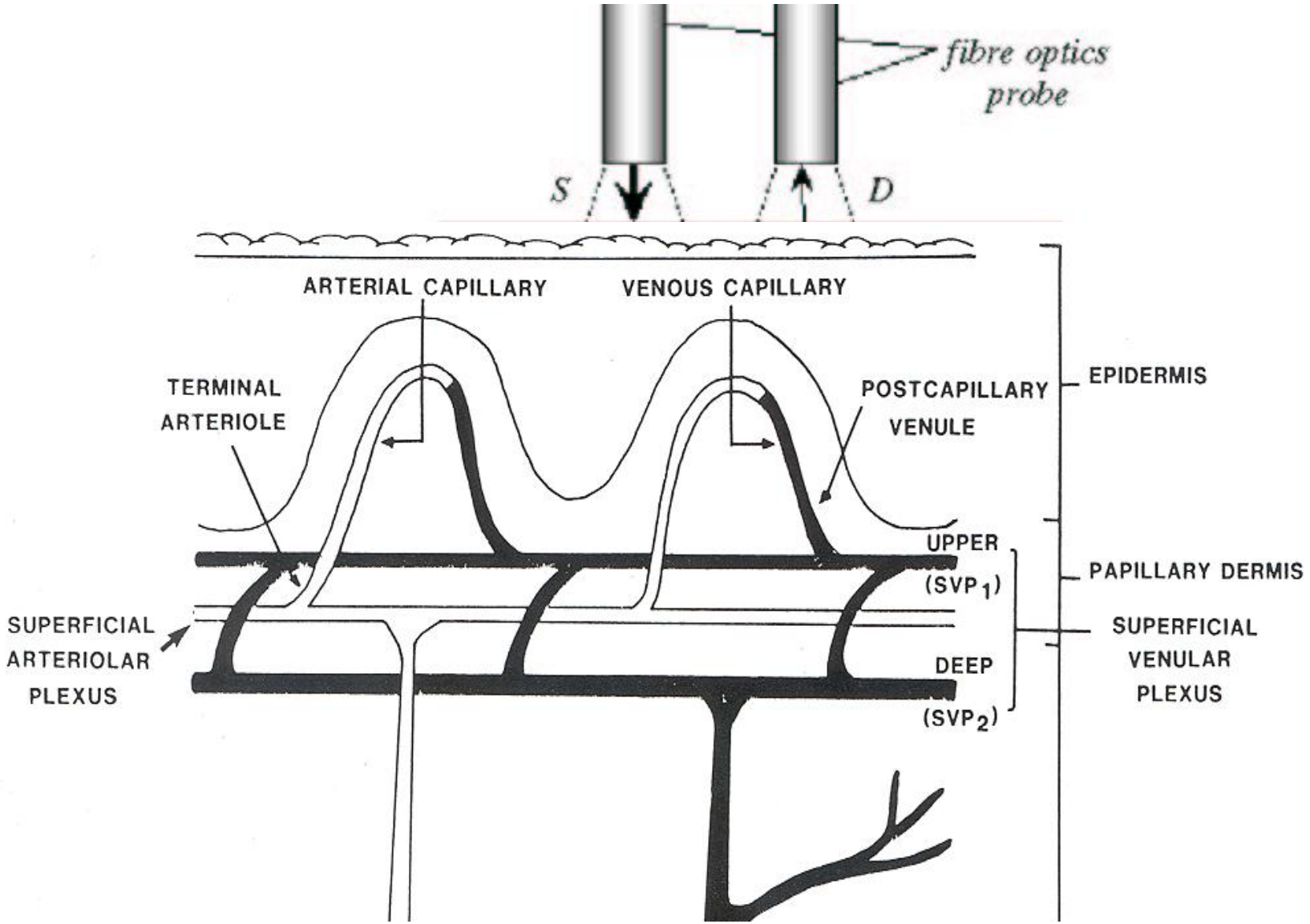


1 – light source; 2 - skin; 3 - detector & PC

Probe


fibre optics probe
S
D
ARTERIAL CAPILLARY
VENOUS CAPILLARY
TERMINAL ARTERIOLE
POSTCAPILLARY VENULE
EPIDERMIS
UPPER (SVP1)
PAPILLARY DERMIS
SUPERFICIAL ARTERIOLAR PLEXUS
SUPERFICIAL VENULAR PLEXUS
DEEP (SVP2)

Probe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PAPILLARY DERMIS
SUPERFICIAL ARTERIOLAR PLEXUS
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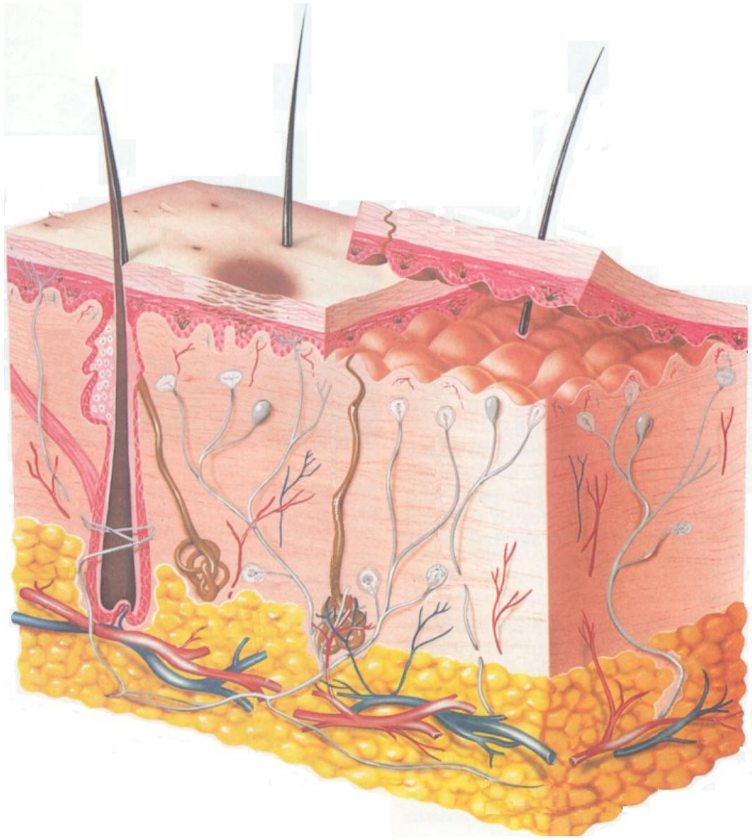
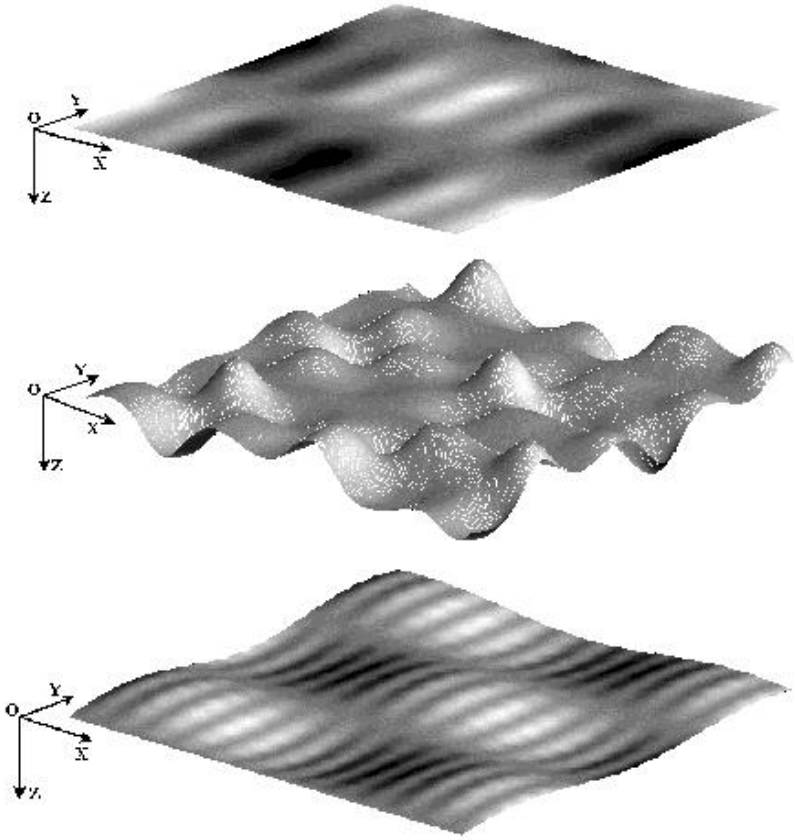
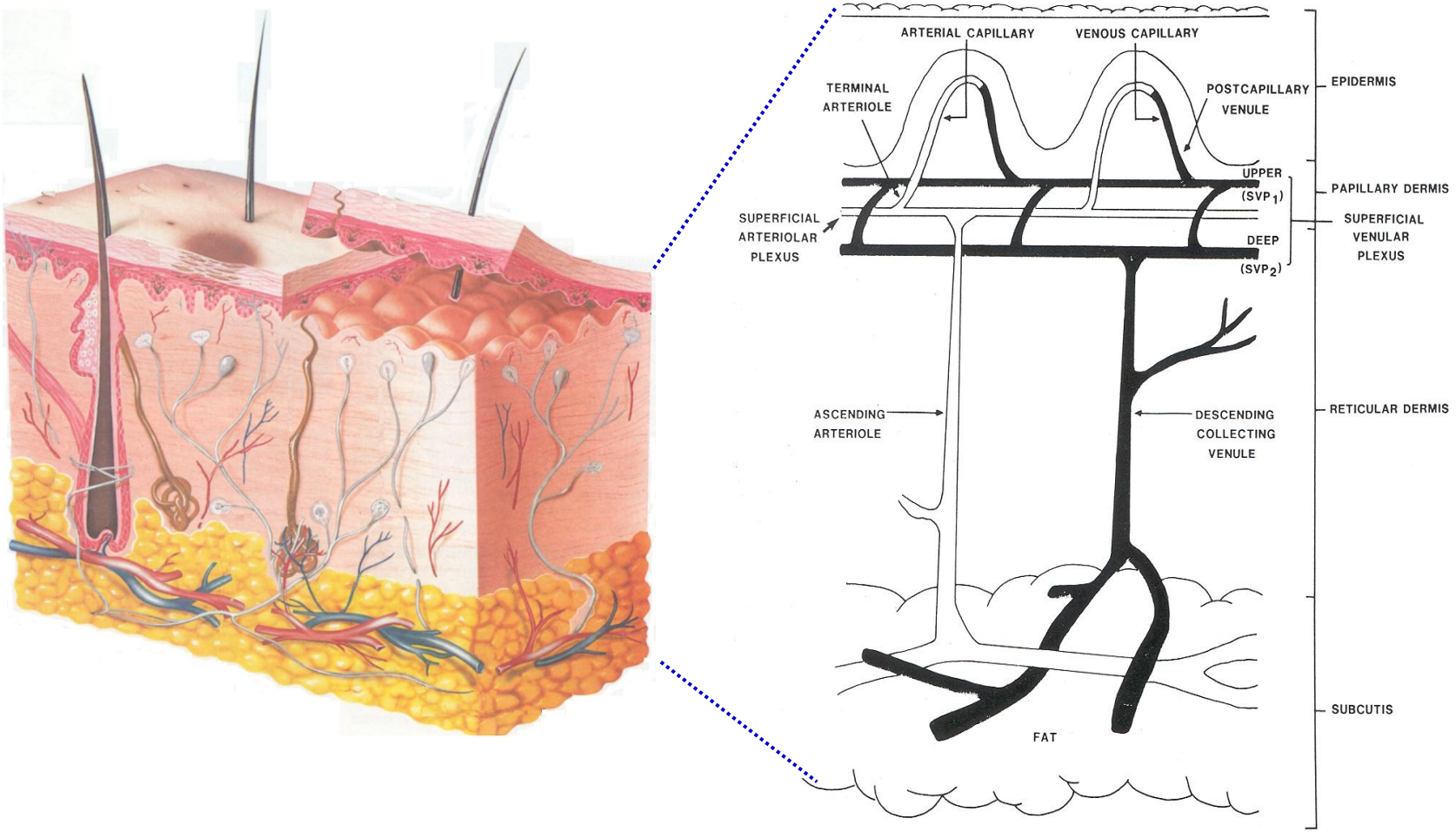
Skin model



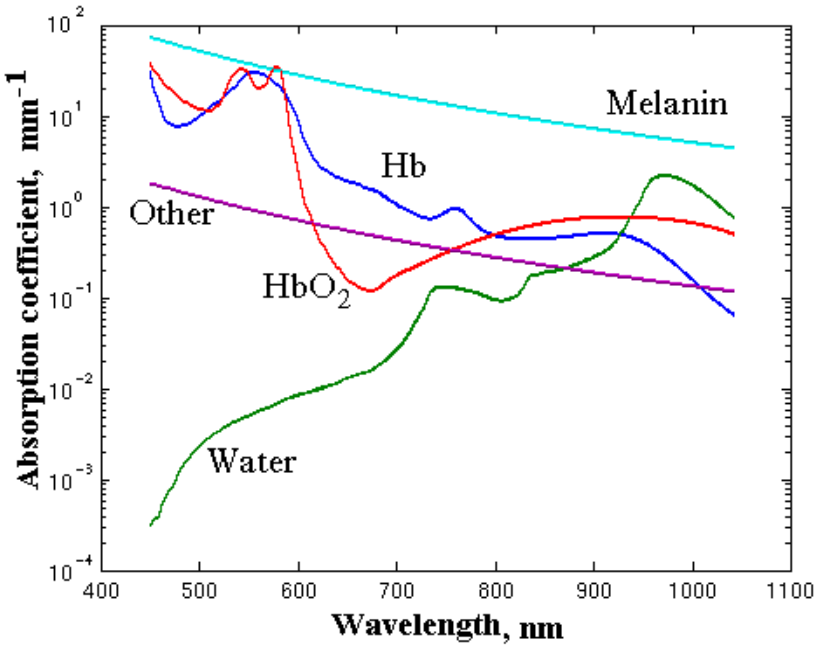


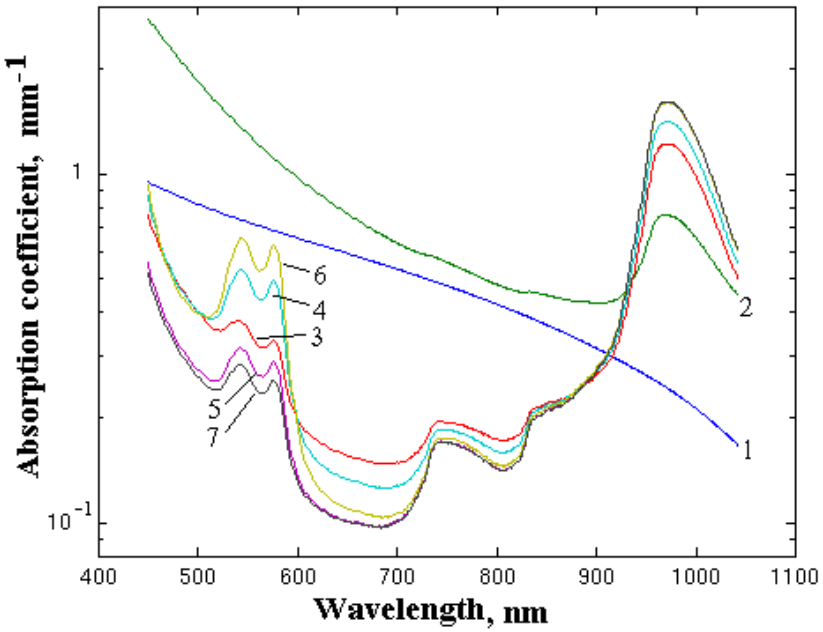
Meglinski, Matcher, *Med. Biol. Eng. Comput.* (2001)

Tissue modeling



Skin optics

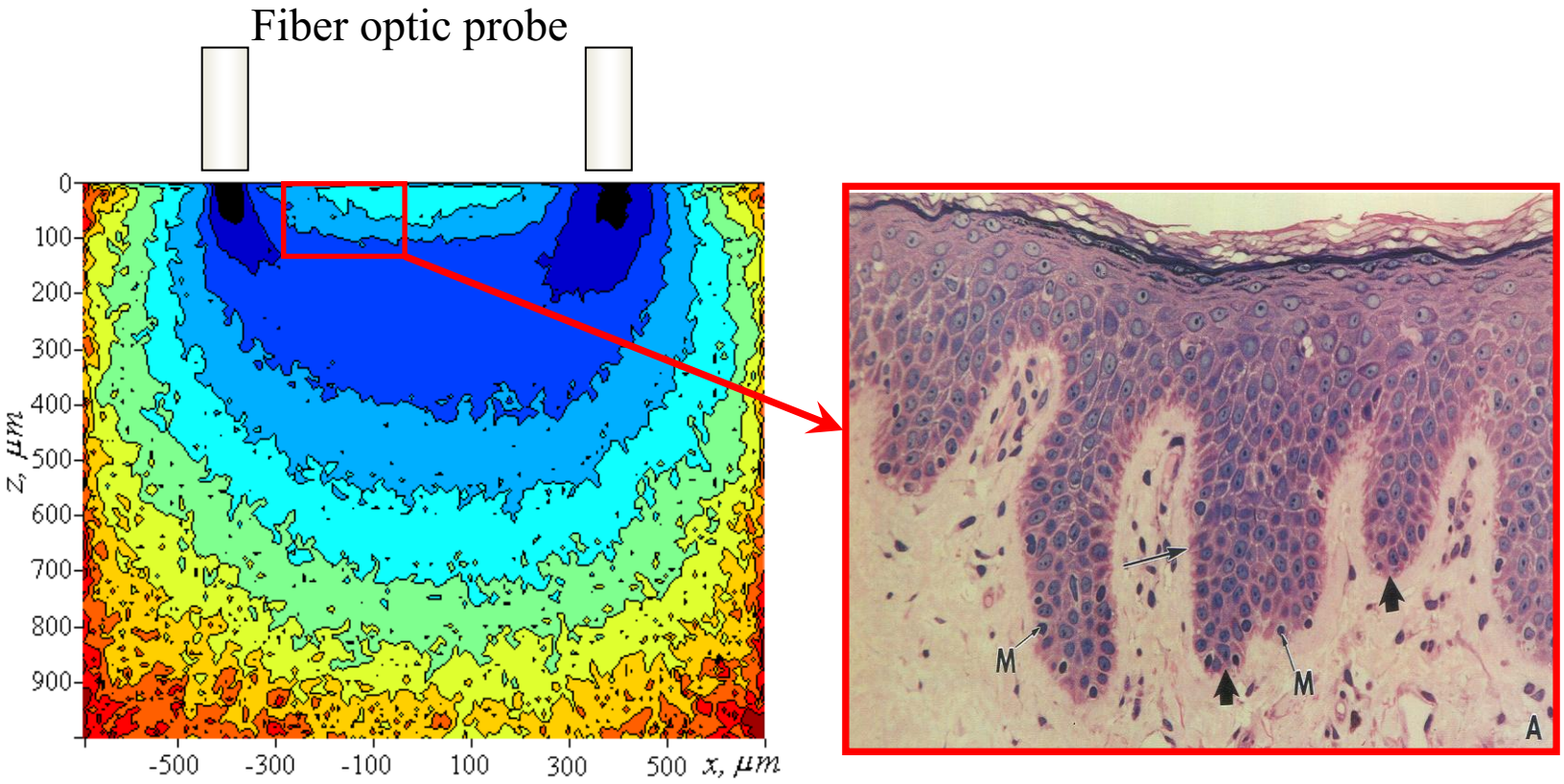




$$\mu_a(\lambda) = \sum_{i=1}^{m} \left(\mu_a^{(i)}(\lambda) C_i \prod_{j=1}^{i-1} (1 - C_j) \right) + \mu_a^{(0)}(\lambda) \prod_{i=1}^{m} (1 - C_i)$$

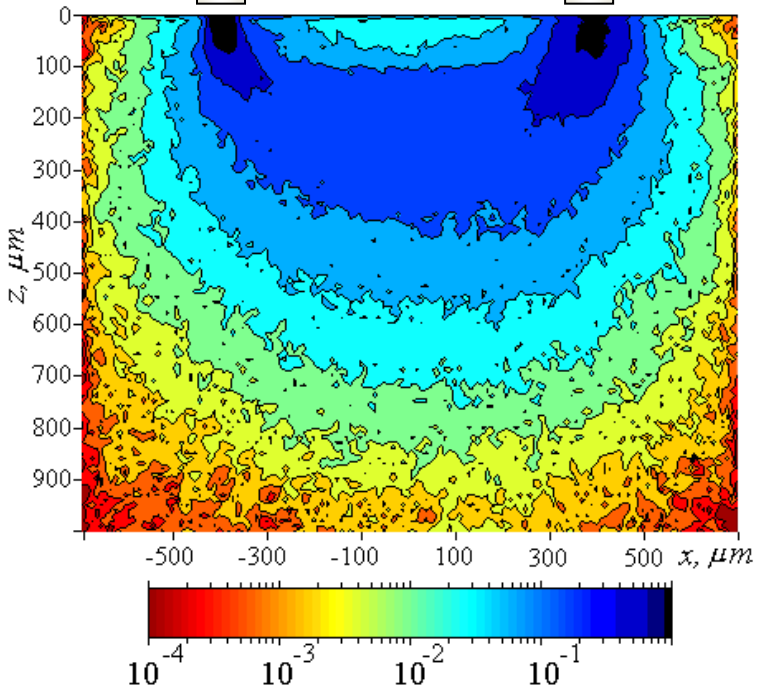
Meglinski, Matcher, *Physiological Measurement*, (2002)

Results of simulation

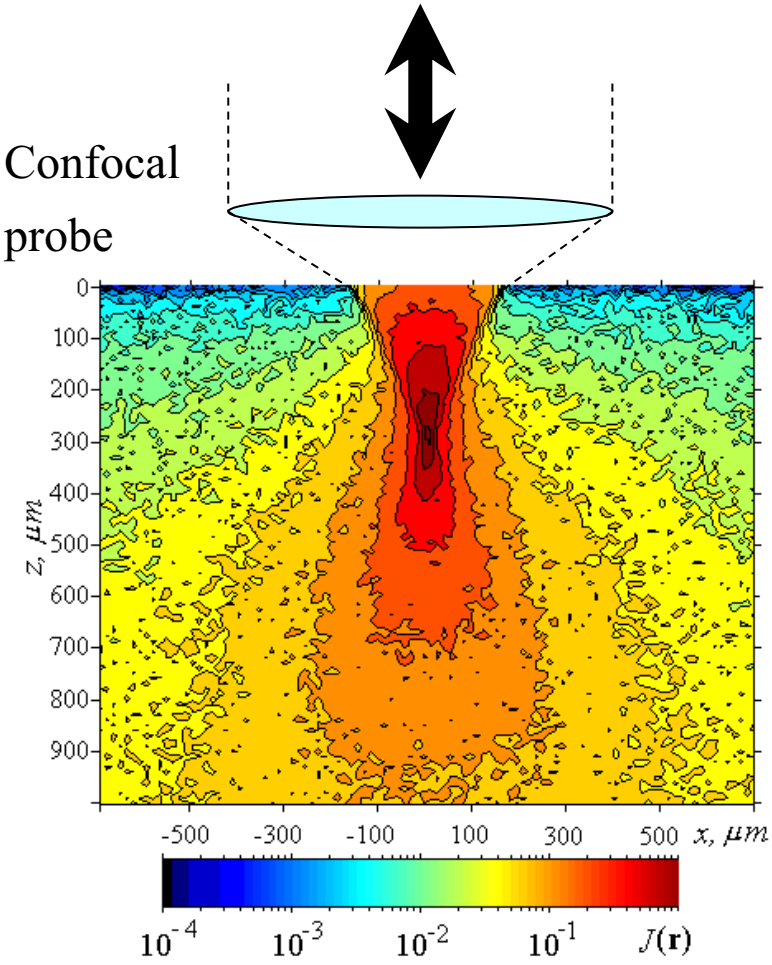


Results of simulation

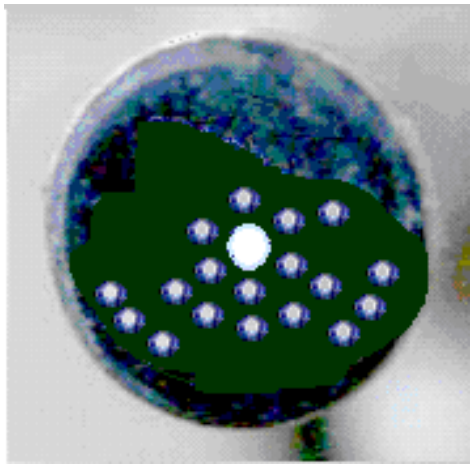
Fiber optic probe

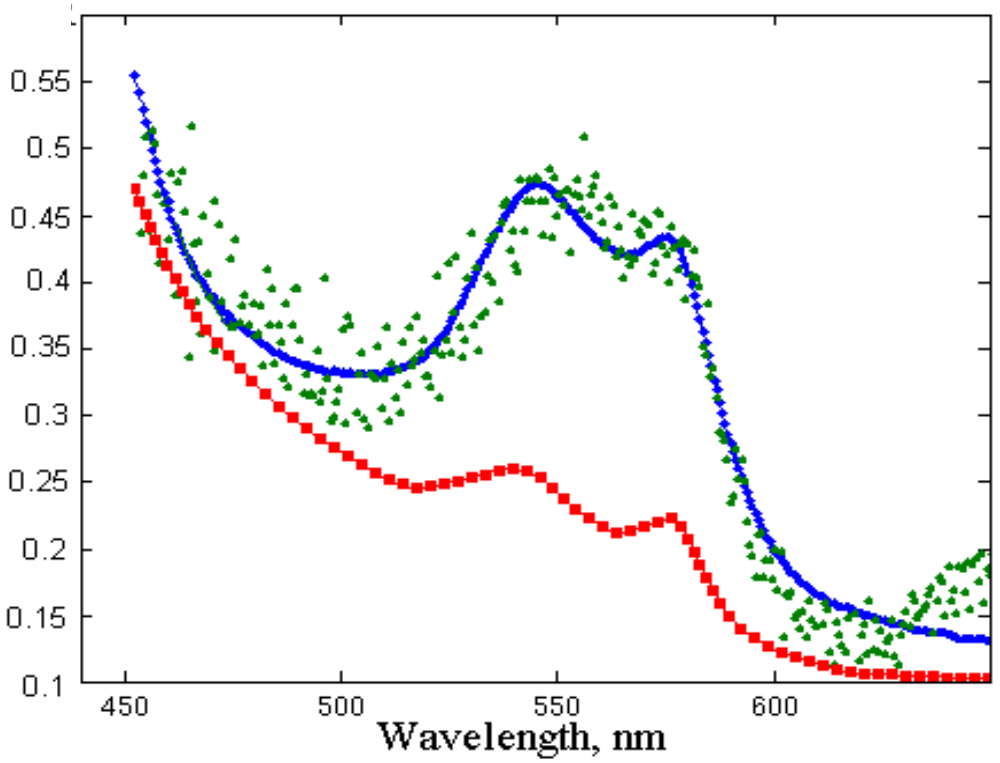


Confocal probe



Results of reflectance spectra simulation



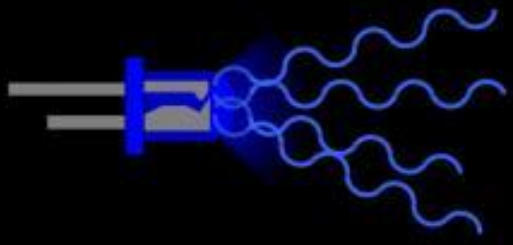


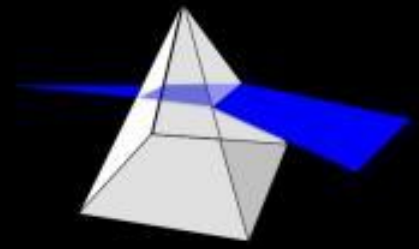
Meglinski, Matcher, *Computer Methods and Programs in Biomedicine* (2002)

Coherence and Polarisation

1

2

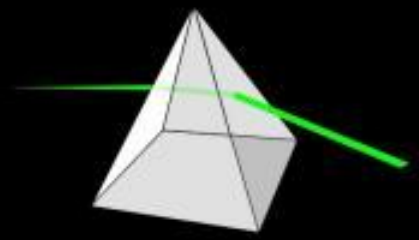




3

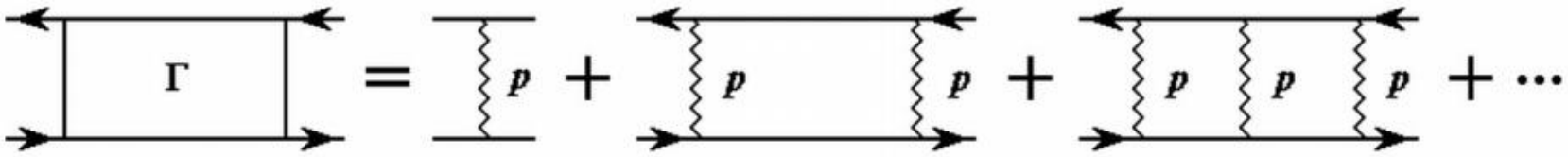
* Cheap lasers loose their coherence at short distance

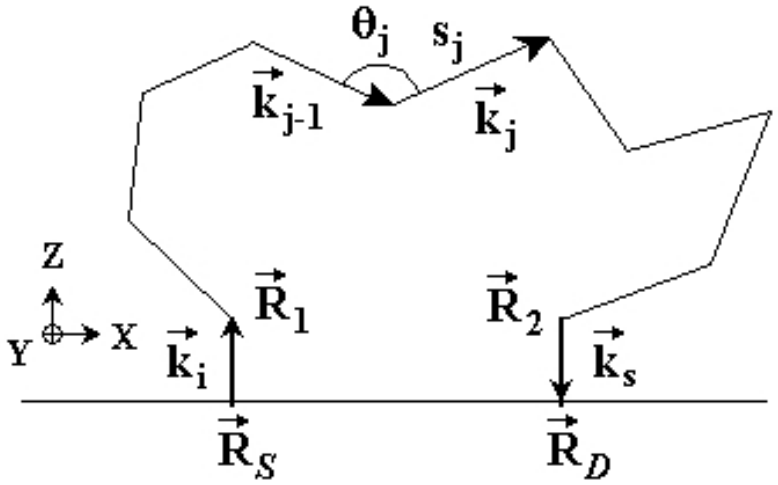
4



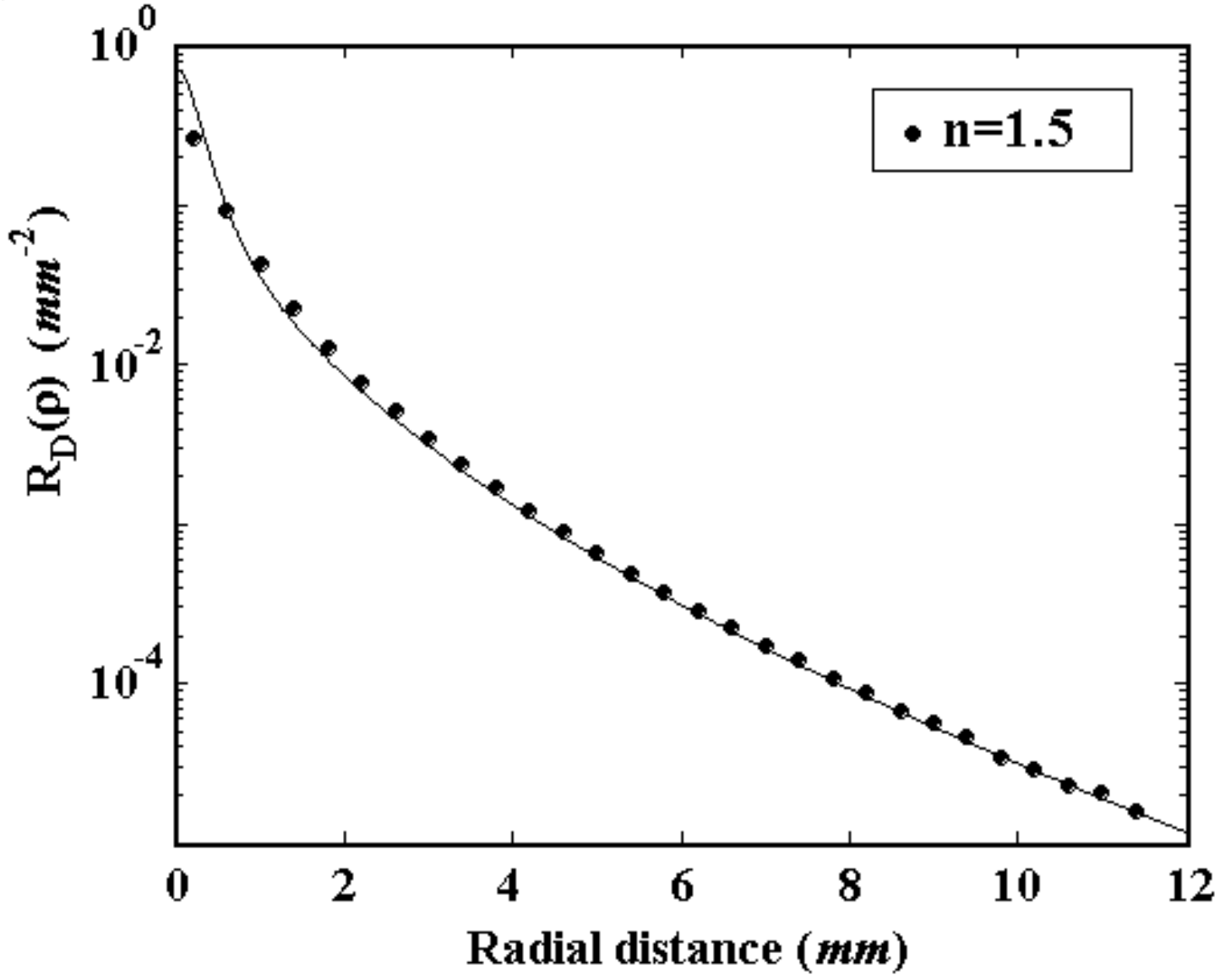
* For holography the laser beam should be coherent and polarized

Bethe-Salpeter Equation vs. Monte Carlo Method

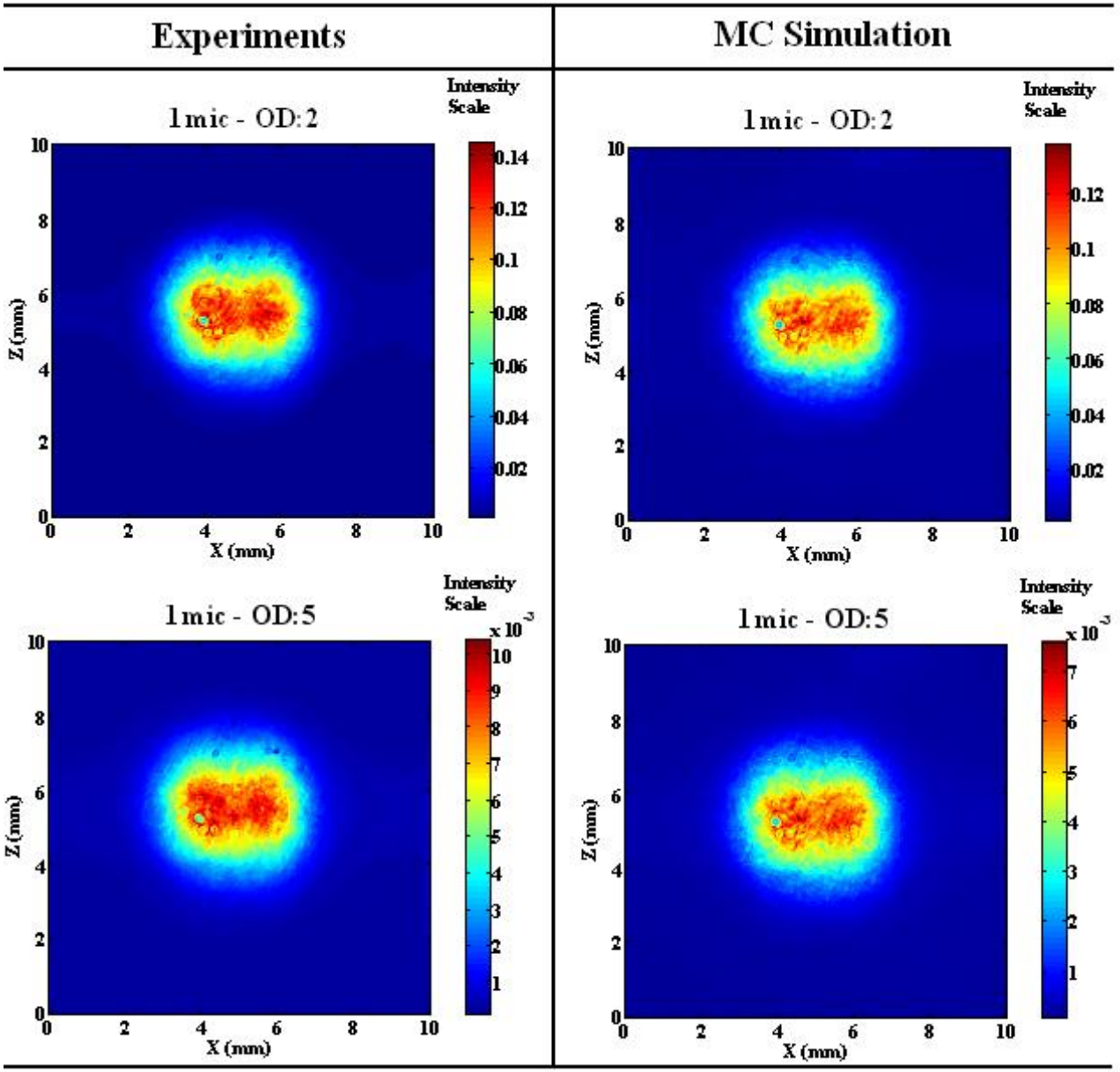




Meglinski, *et al. Proc. Roy. Soc. A* (2005)

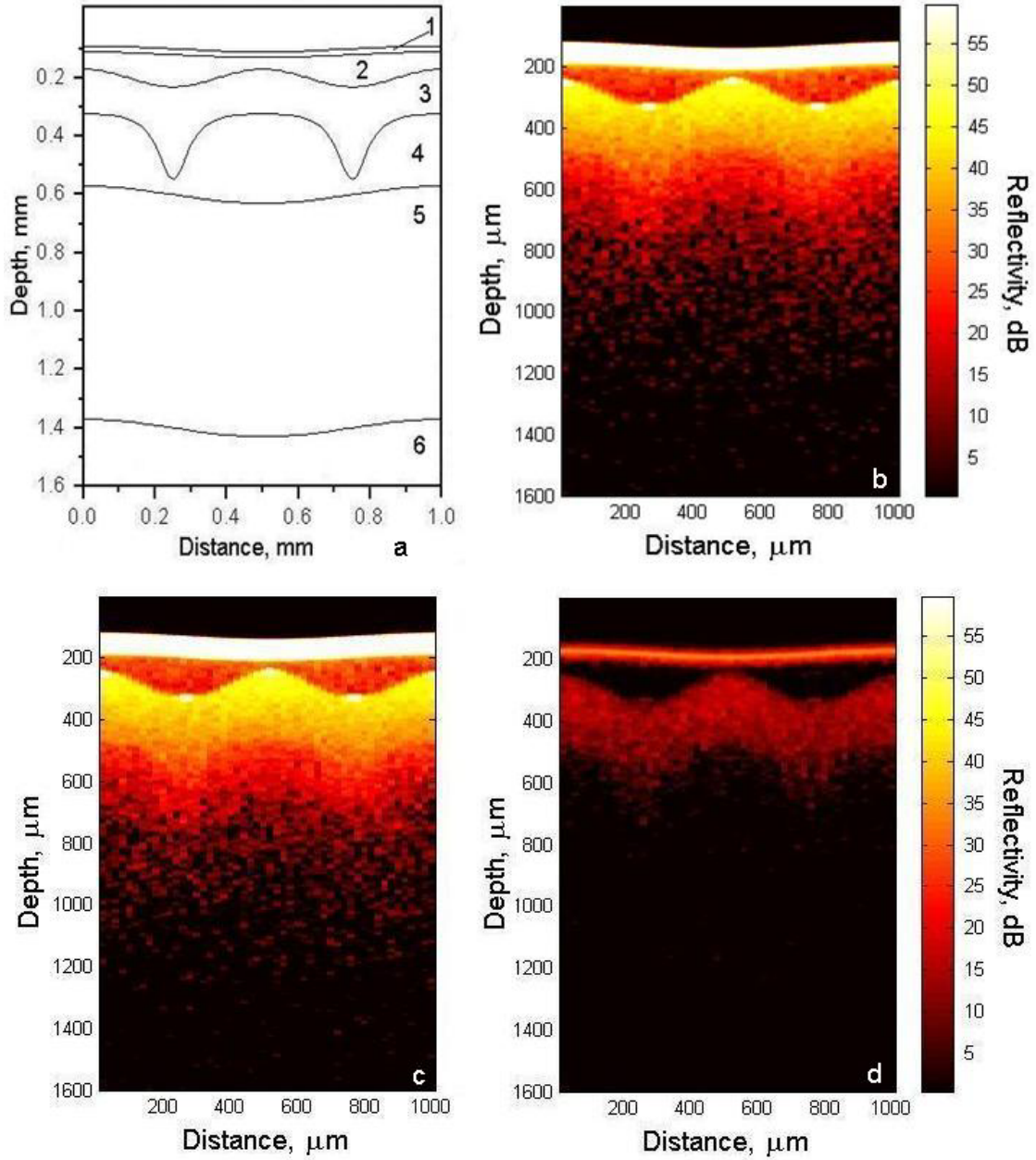


$$R_{\mathrm{D}}(\rho) = \int_{2\pi} d\Omega [1 - R(\theta)] \frac{1}{4\pi} \left[\Phi(\rho) + 3D \frac{\partial \Phi(\rho)}{\partial z} \cos\theta \right] \cos\theta$$



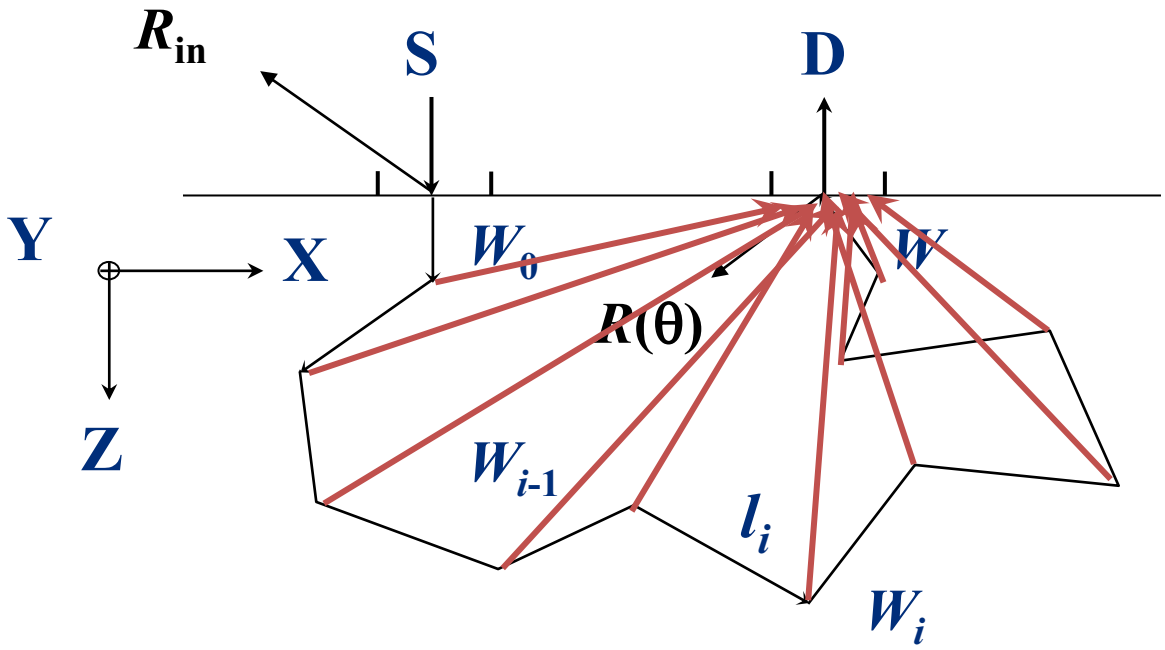
Berrocal, et al, *Laser Phys. Lett.* (2006)

Results of OCT Images Simulation



Meglinski, et al, *Optics Letters* (2008)

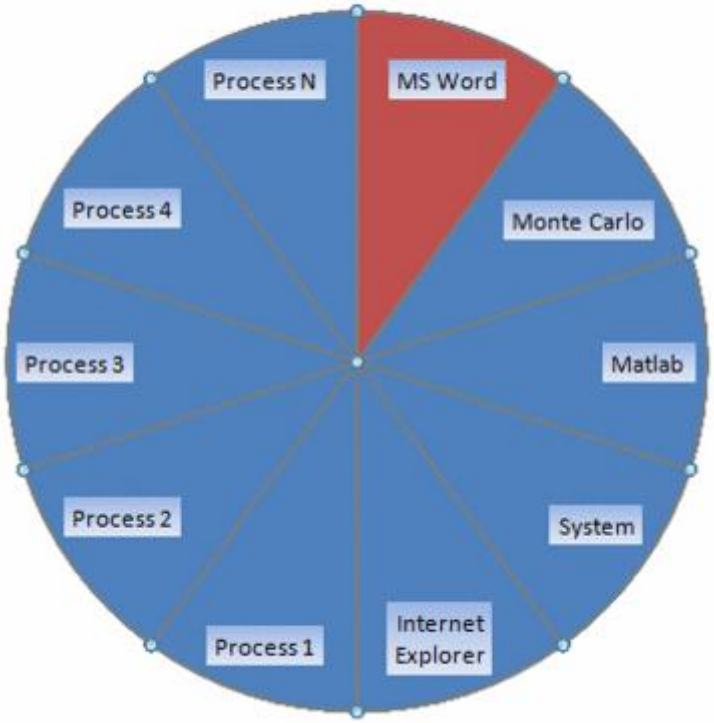
Method Monte Carlo



- μ_s, μ_a
- $l_i = - ln(\xi)/ \mu_s$

$$W = \underbrace{\left(1 - R(\theta_i)\right) W_0 \left[\prod_{p=1}^{M} R(\theta_i)\right]}_{1} \underbrace{\exp\left(-\sum_{i=1}^{N_j} \mu_a l_i\right)}_{2}$$

Computing Monte Carlo on a regular CPU

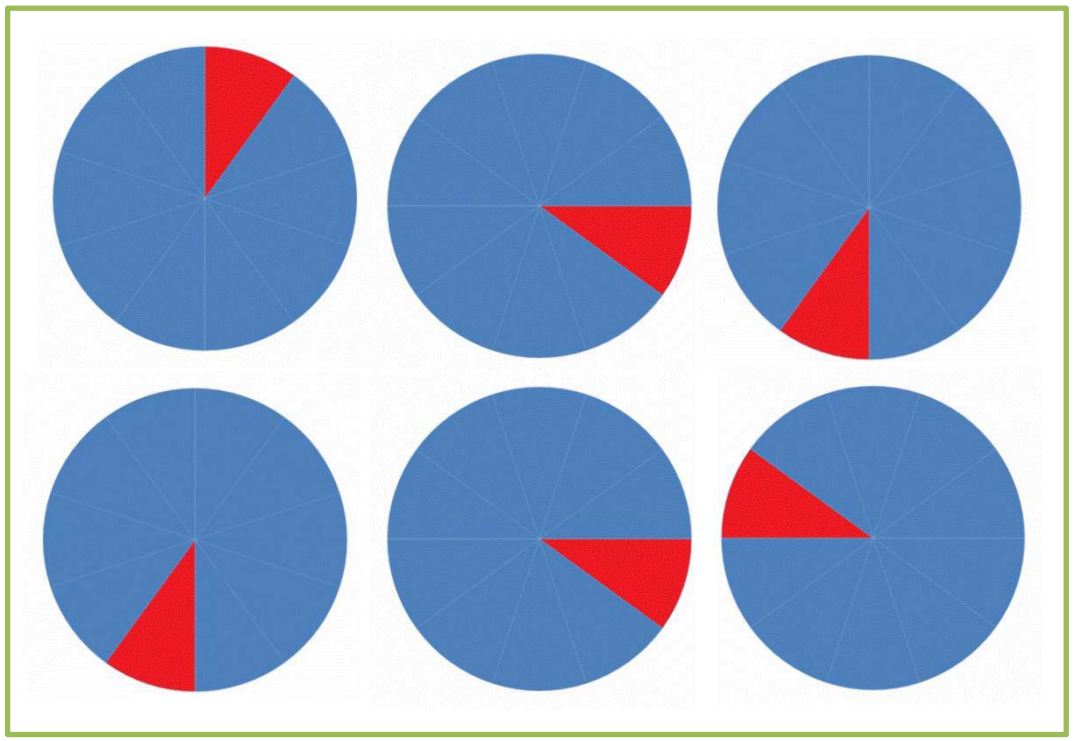


A single core CPU is:

1. MIMD architecture (multiple instructions / multiple data)
2. Executing various instructions for various processes
3. Switching context so every process could perform its operations
4. Fast execution of one thread at one time slice
5. CPUs have been designed for a wide range of common applications

Average detection time of a single photon: 50-100 ms

Computing Monte Carlo on a multi-core CPU



A multiple core CPU is:

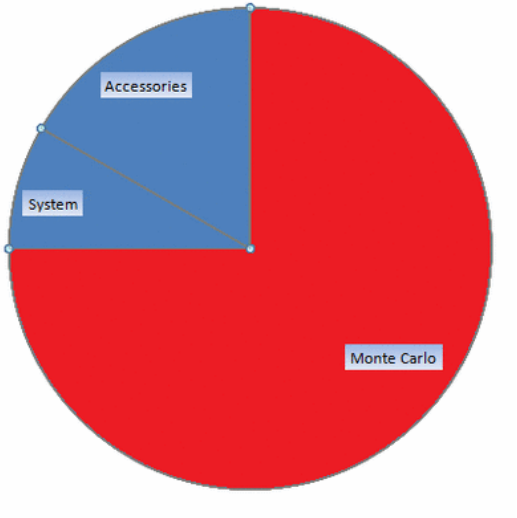
1. Up to 6 independent MIMD architecture cores in one unit
2. Each process executes on its own core
3. Switching context in cores so every process could perform its operations
4. Fast execution of a number of processes at one time slice
5. The large boost in performance for applications

Average detection time of a single photon: 10-20 ms

Monte Carlo optimisation and parallel computing on a CPU

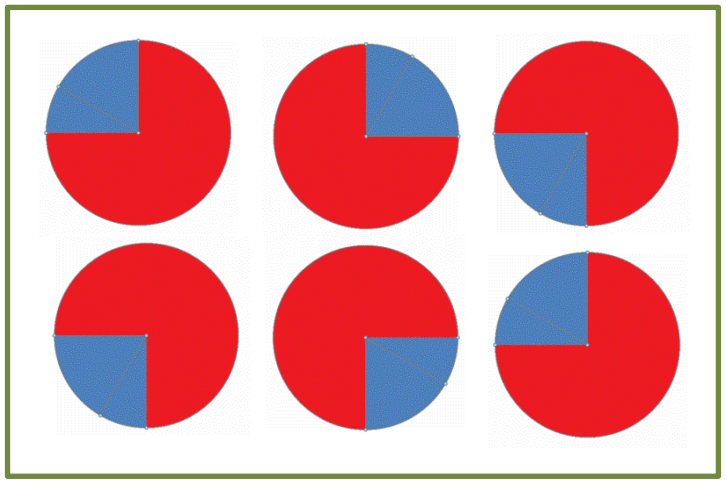
1. Optimizing the algorithm
2. Optimizing the source code
3. Creating a number of threads executing on the CPU
4. Performing Monte Carlo simulation as a high-priority task
5. Running Monte Carlo simulation at the operating system level

A single core CPU



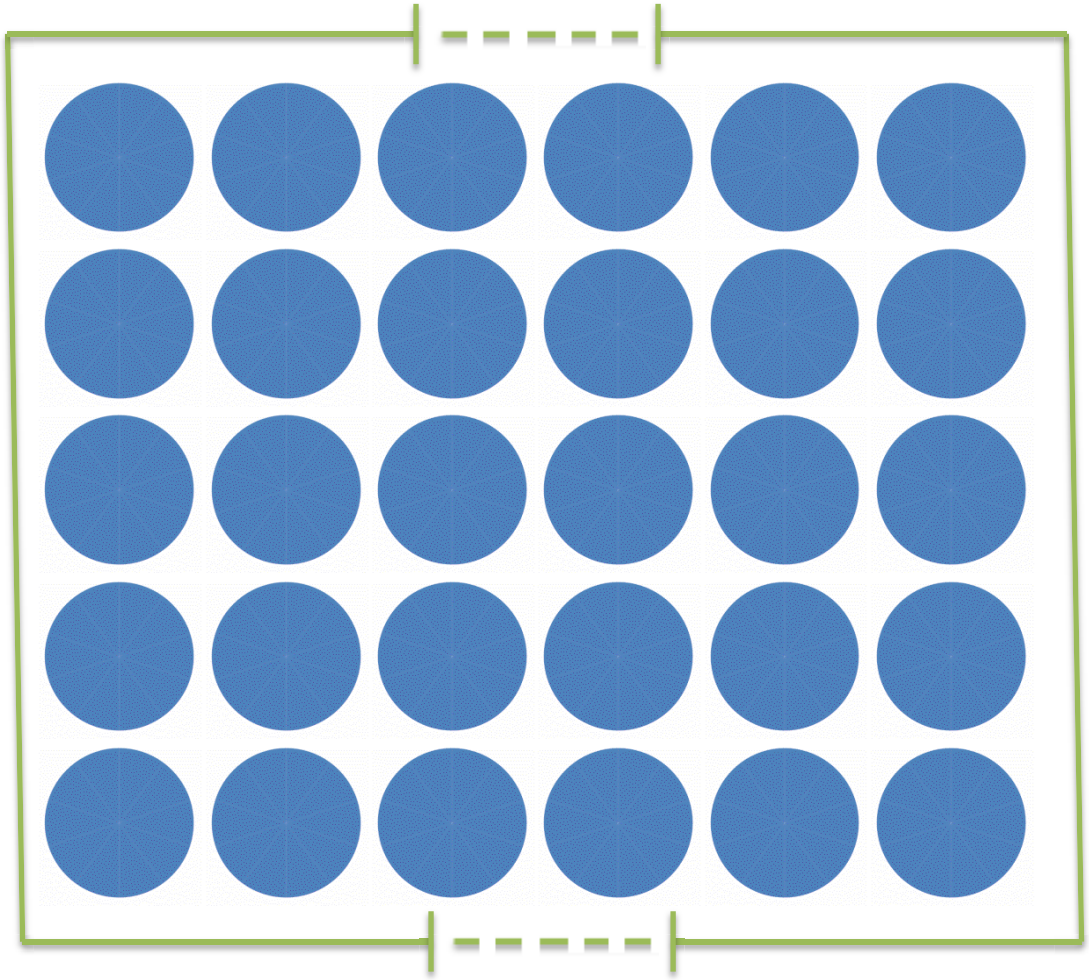
Average detection time of a single photon: 7-10 ms

A multi core CPU



Average detection time of a single photon: 0.1 – 1 ms

Monte Carlo parallel computing using NVIDEA CUDA

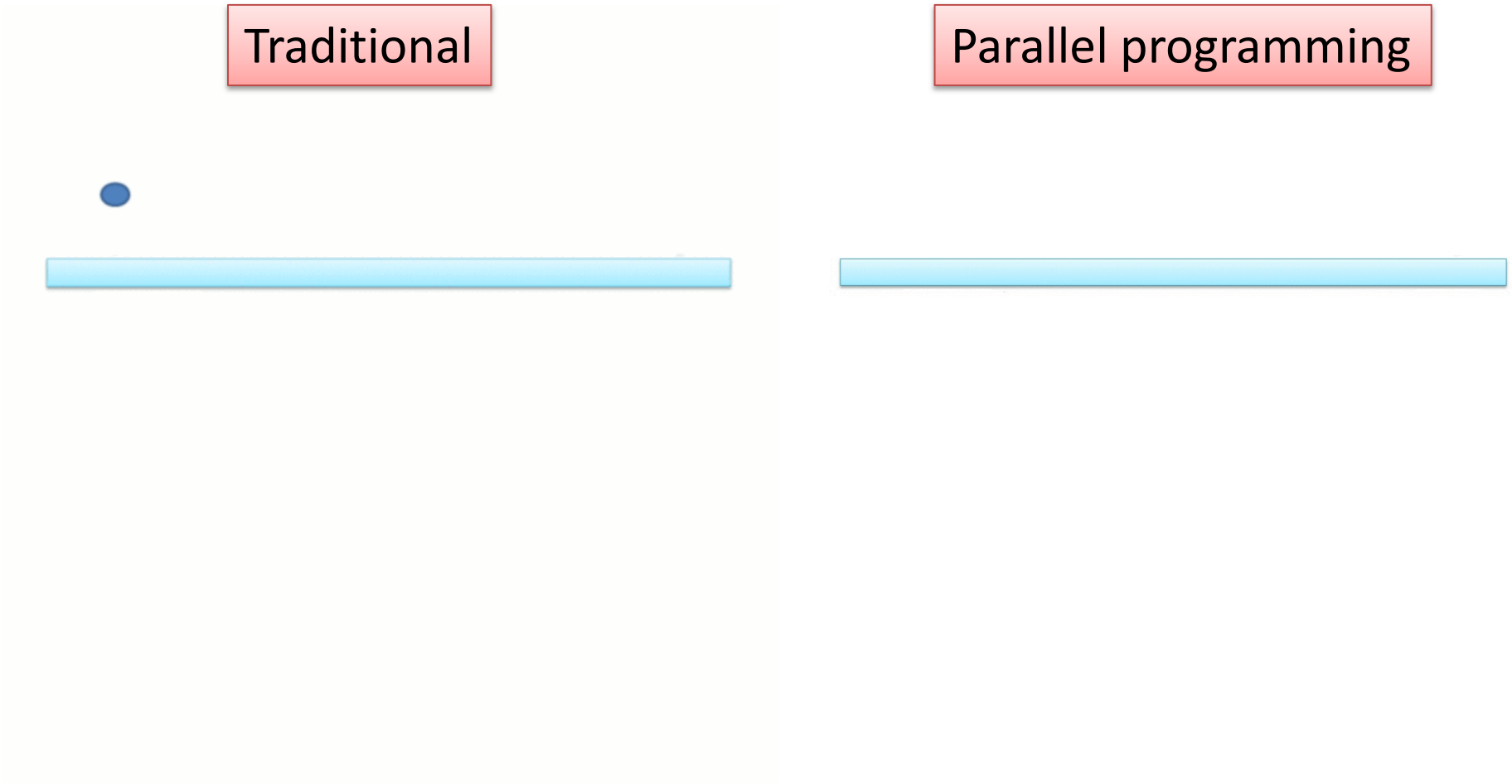


A NVIDEA CUDA GPU is:

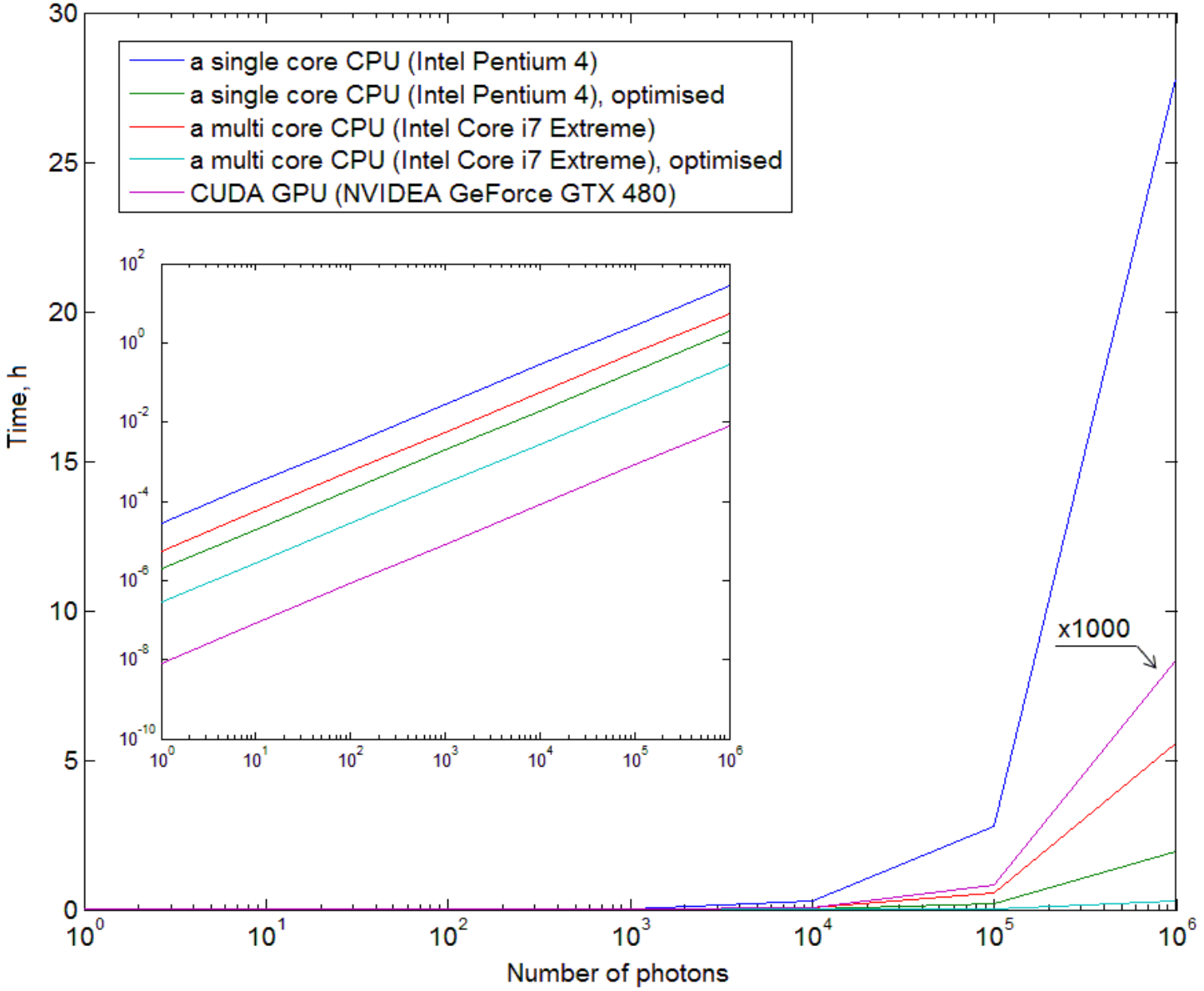
1. Compute Unified Device Architecture
2. Up to 60 independent SIMD (single instruction / multiple data) architecture cores in one unit
2. Up to 480 CUDA cores able to execute thousands of MC threads simultaneously
4. No context switching, extremely fast GDDR5 memory
5. Optimized linear algebra and graphics libraries
6. Support of Object Oriented Languages and modern development approach

Average detection time of a single photon: 60-120 µs

Photon random walk using the traditional and parallel programming approaches

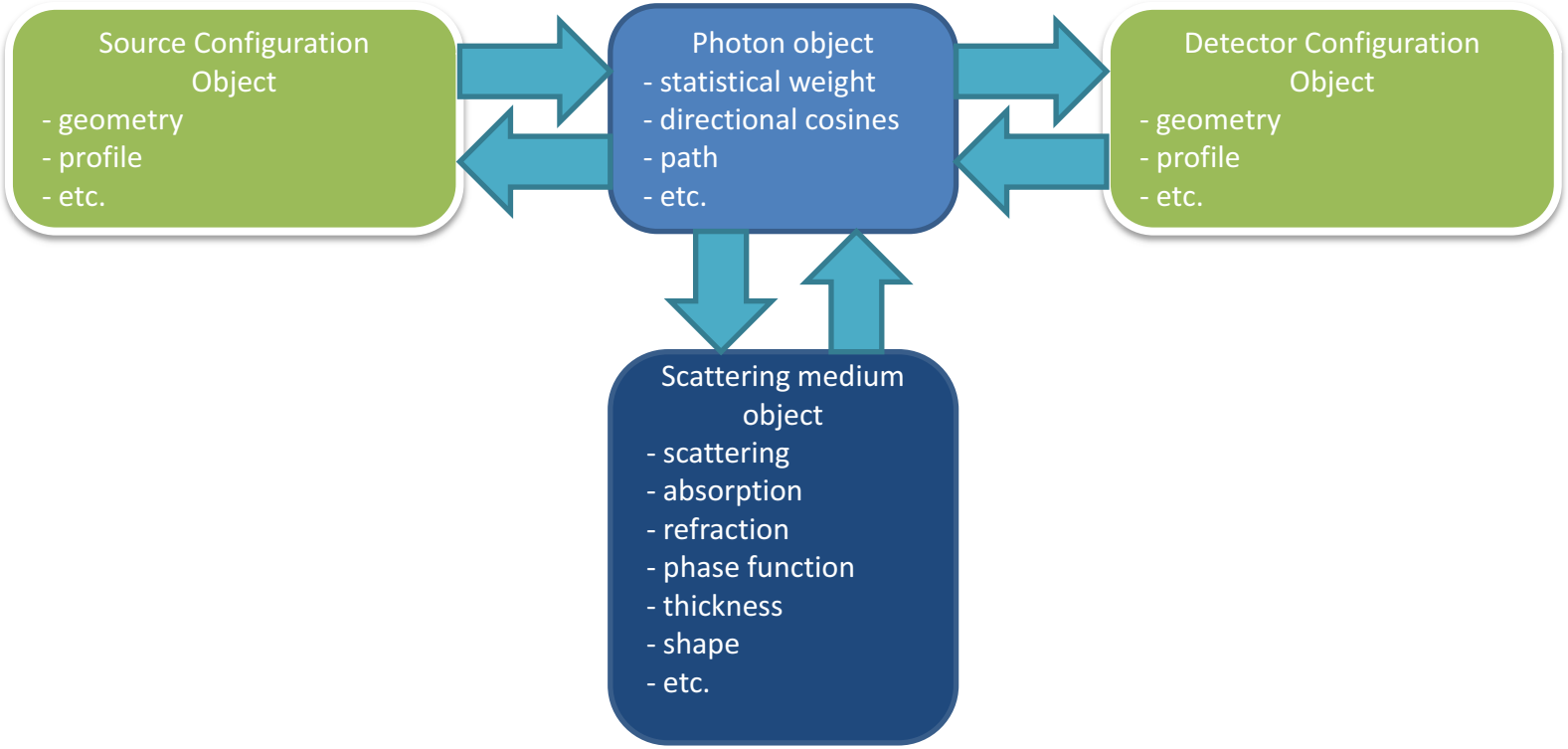


Monte Carlo modelling compared performance



Object Oriented Programming approach in the Monte Carlo modelling

The unified Monte Carlo modelling core

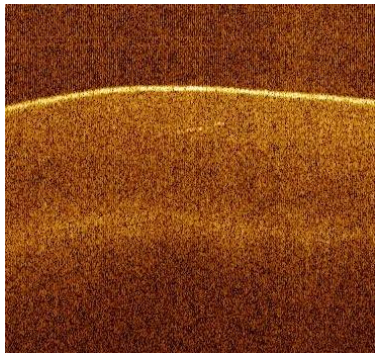


1. Creation of objects describing: the nature of optical radiation, media structure, probe configuration
2. Objects interacts according to laws of physics: scattering, absorption, reflection, polarisation
3. Developing a unified complex modelling system utilizing OOP features: abstraction, encapsulation, polymorphism, modularity
4. Optimized modelling performance and bottlenecks with NVIDEA CUDA

Further development of the Monte Carlo modelling

Interoperability with OCT / Imaging systems

1



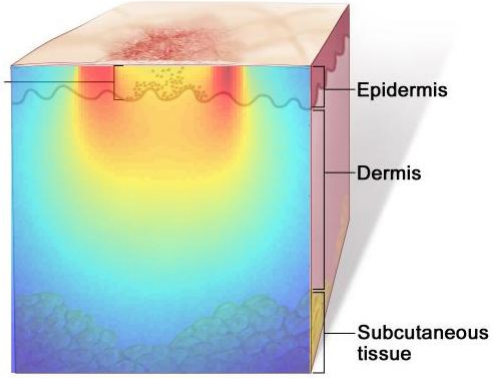
2

Imaging Module

3

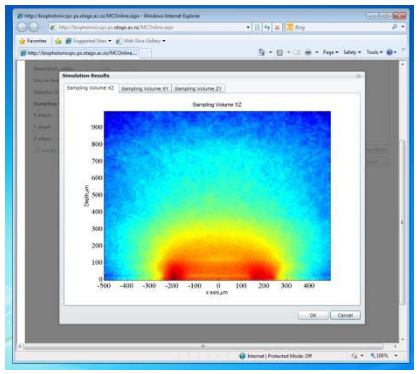
Monte Carlo Modelling System

4



1. Acquisition OCT imaging data with Swept Source Optical Coherence Tomography System
2. Exporting imaging data in Monte Carlo modelling software
3. Proceeding imaging data into a complex computational sample within the imaging module
4. Performing Monte Carlo simulation

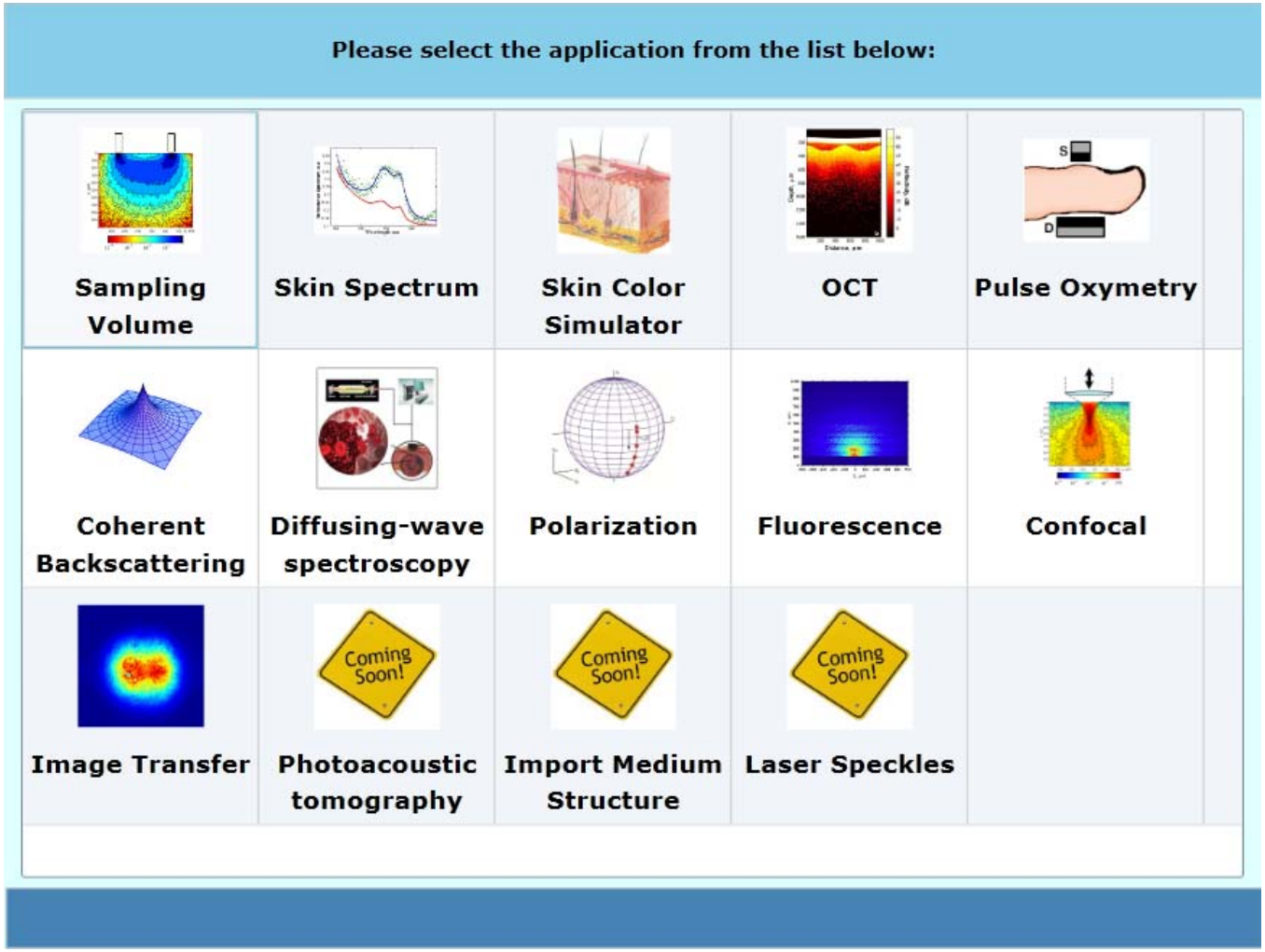
Monte Carlo - Online Solution



Website Server CUDA GPUs

- NVIDEA CUDA GPUs is the heart of MC that performs all highly-intensive computations
- The server processes requests, manages resources and controls GPUs
- Online Solution utilizing Microsoft Silverlight technology provides user friendly access to the Server and produces MATLAB-based paper style outcome in a few seconds

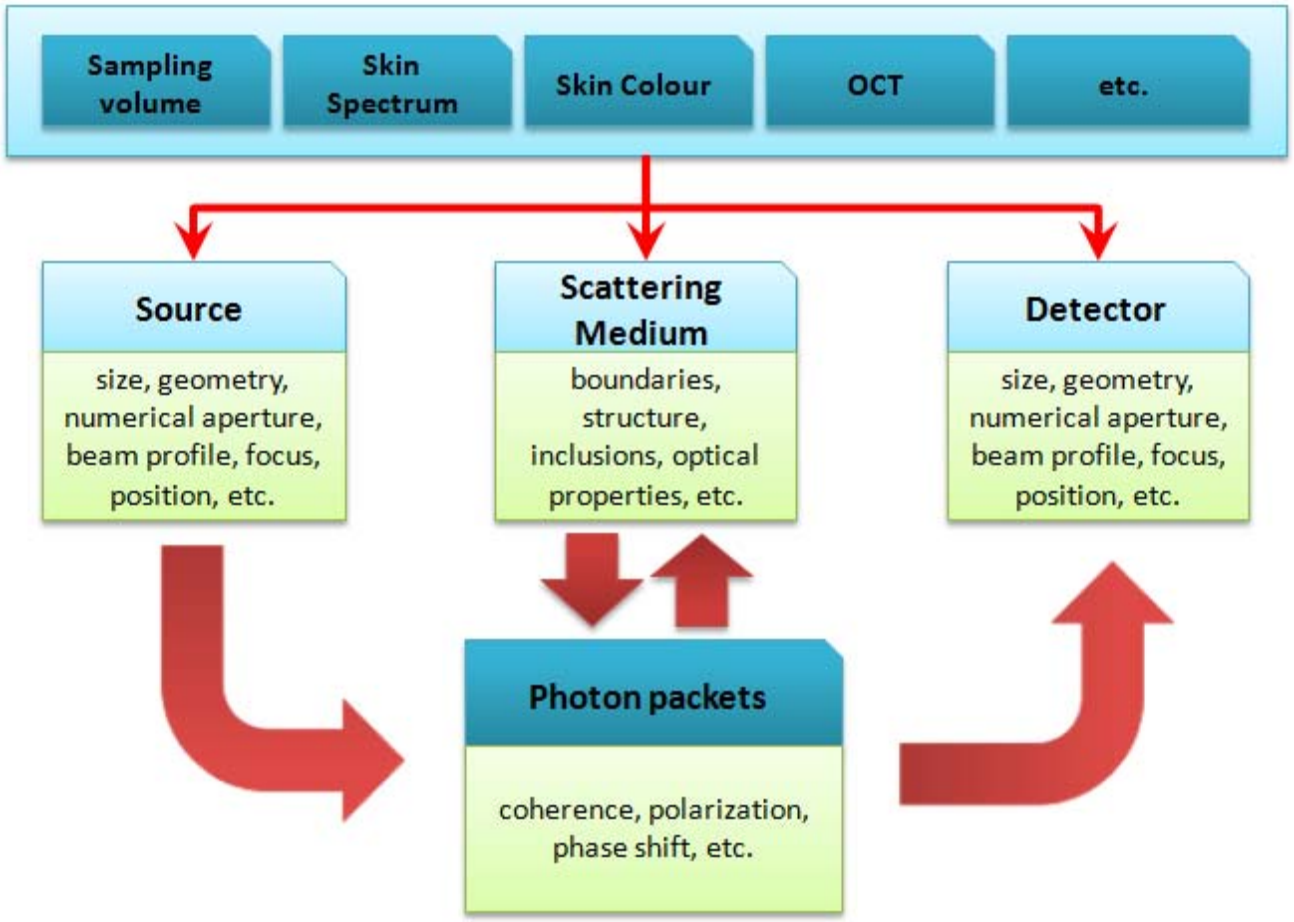
Online GPU-accelerated multipurpose Monte Carlo simulation tool



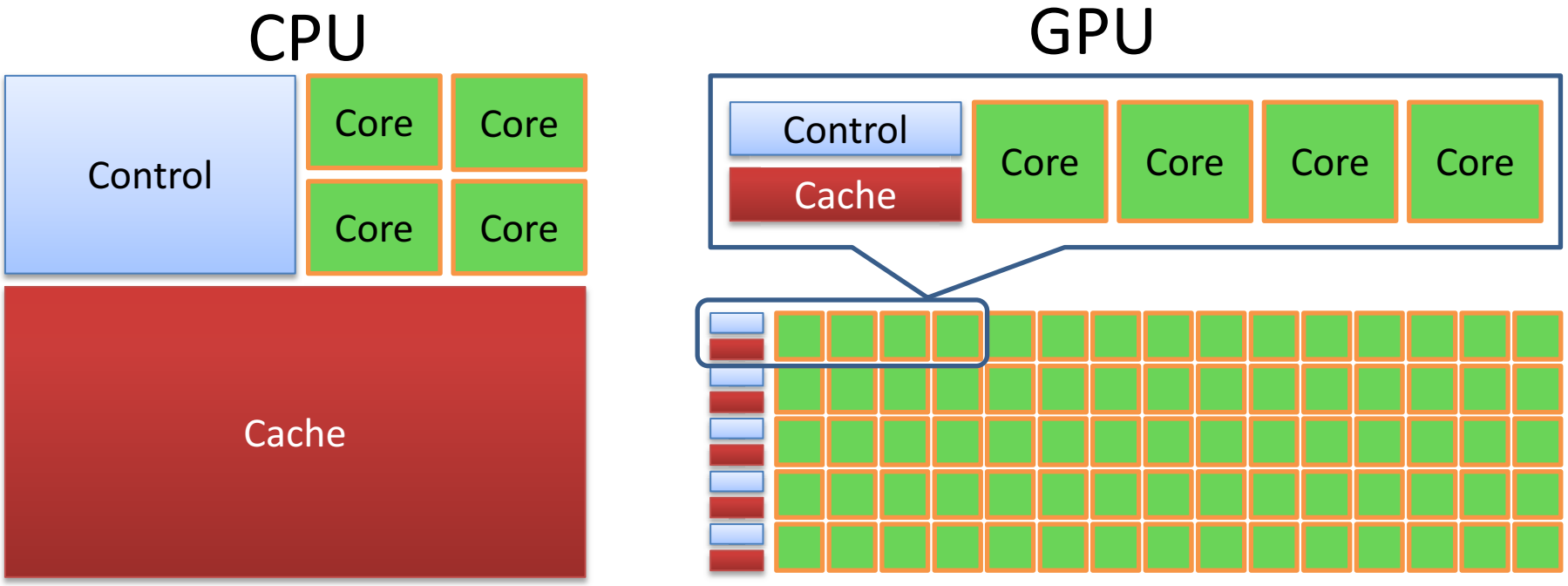
The Concept

- The web frontend is accessible from anywhere, a capable web browser is the only requirement. It accepts requests for MC simulations and provides users with results
- The server processes requests, manages resources and controls the GPUs
- The GPUs perform the highly-intensive MC simulations bringing a massive speedup (1000x).

Generalized object-oriented MC model structure



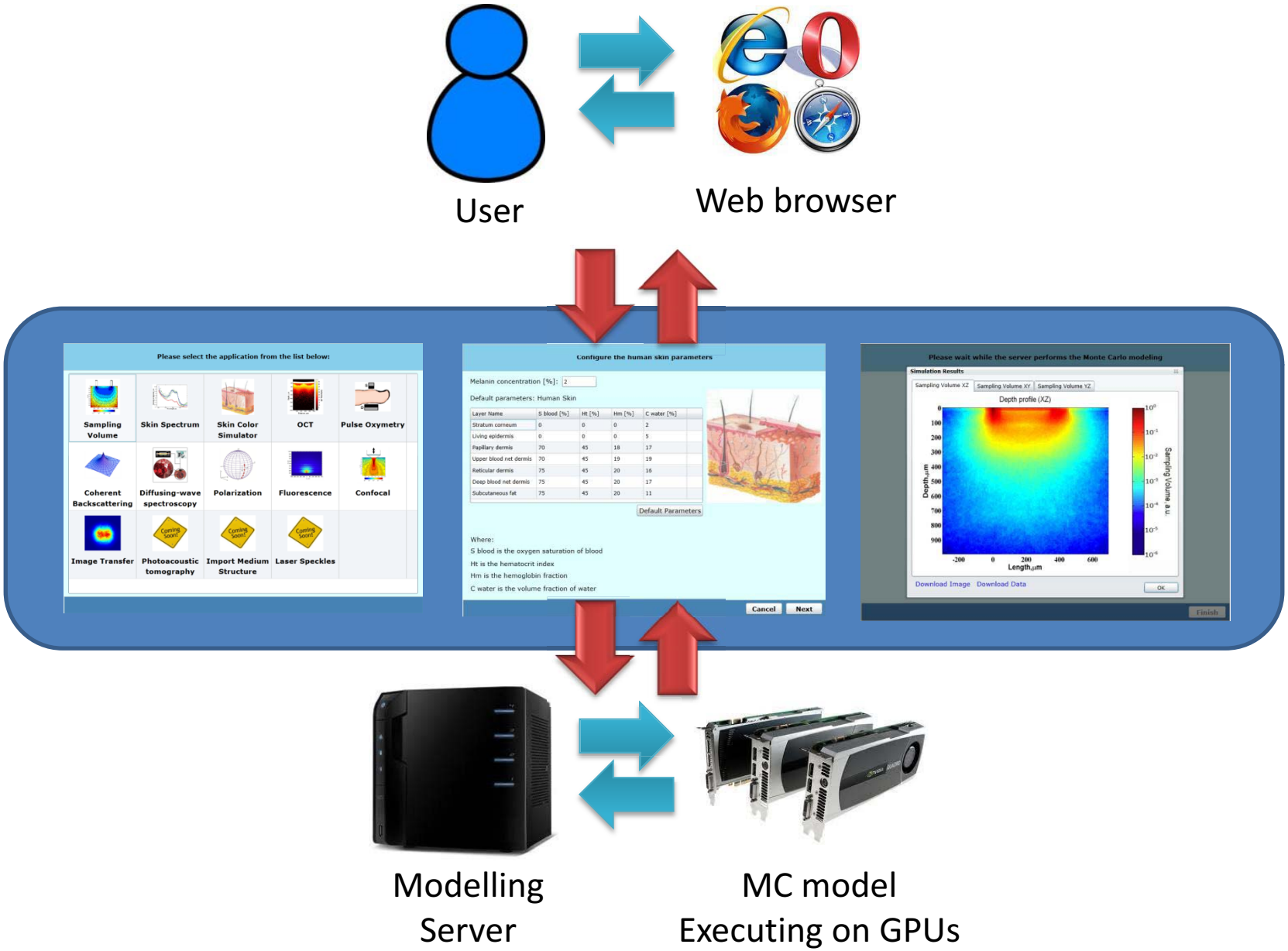
CUDA acceleration of the MC model



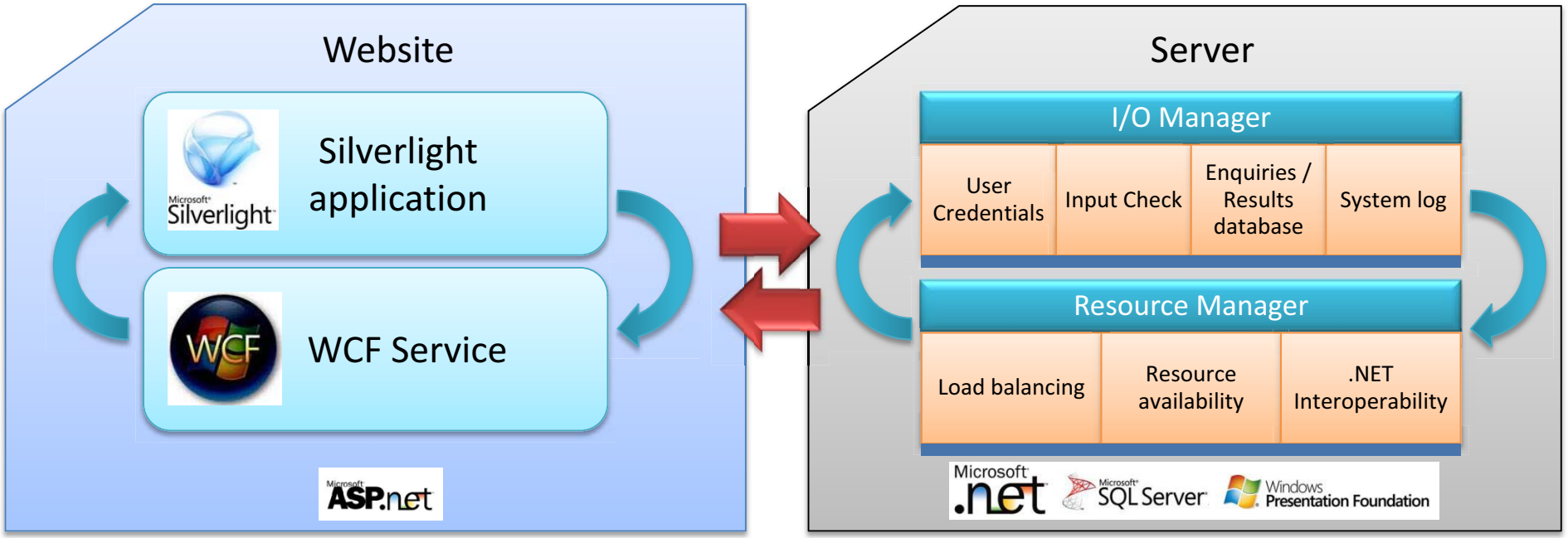
1. CUDA is an acronym Compute Unified Device Architecture, a parallel computing technology by NVIDEA Corp.
2. Hundreds CUDA cores able to process thousands of MC photon packets simultaneously
4. No context switching, extremely fast GDDR5 memory
5. Optimized linear algebra and graphics libraries
6. Support of Object Oriented Languages and modern development approach

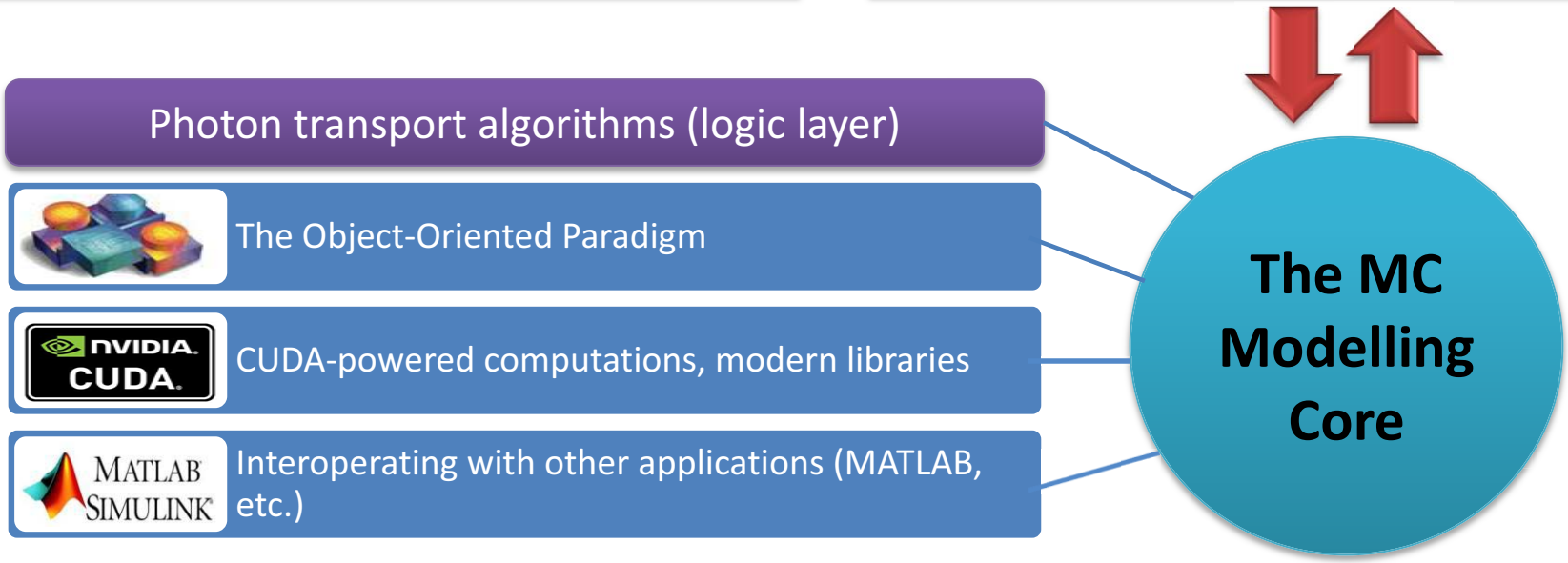
From hours and days to seconds and minutes…

Online Solution: Thin client model



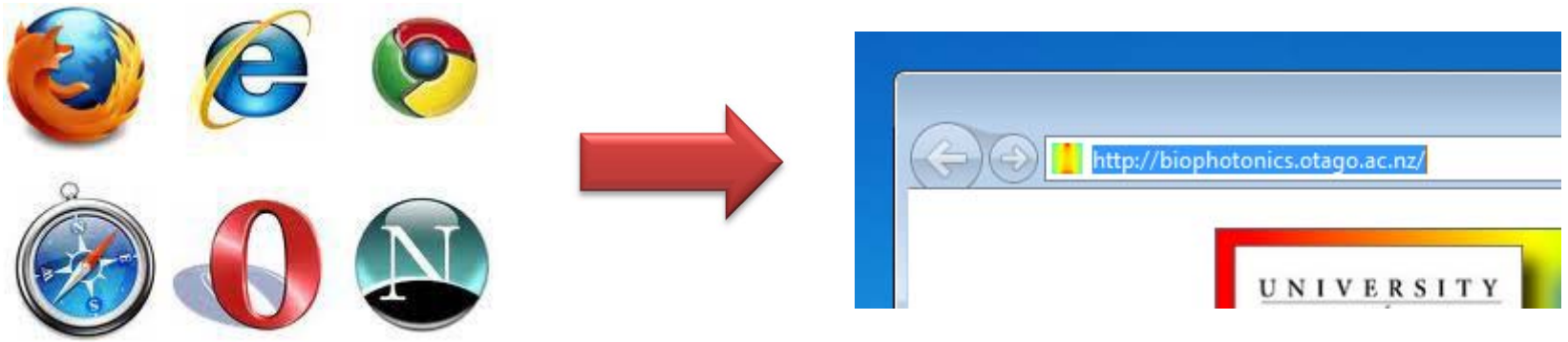
Technical details: Close Look





Accessing the Tool

1. Open you favourite web browser and type http://biophotonics.otago.ac.nz/ in the address bar



1. Chose the tab named “Monte Carlo Online” on the top menu to load the Monte Carlo web application.

Using the Tool

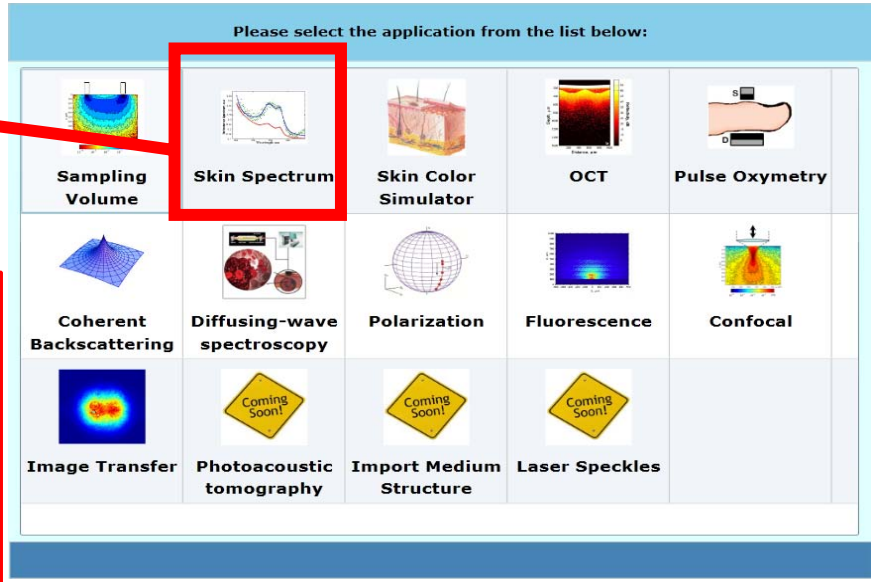
1. Select the desired application by clicking the corresponding icon

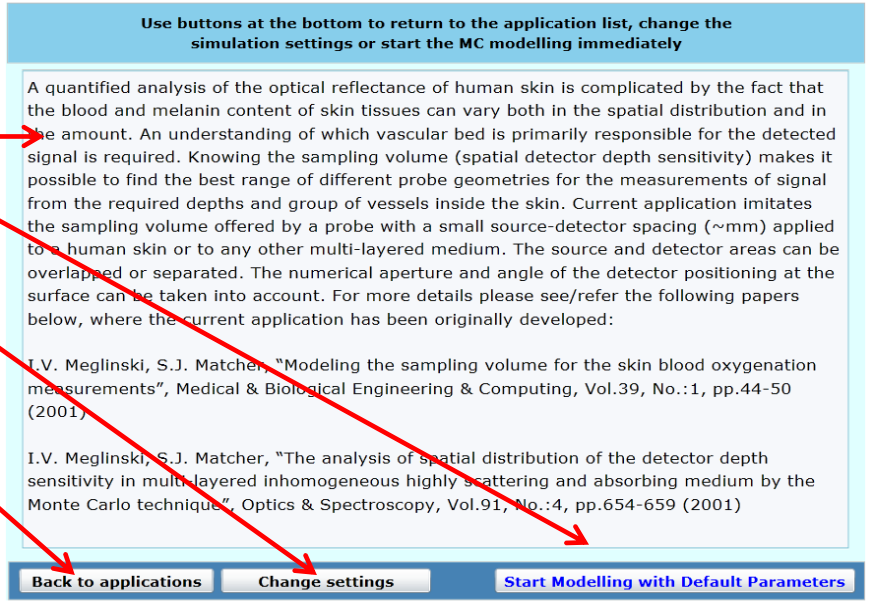
2. The application description will appear, from that point MC user can:

a) start modelling with default parameters

b) change modelling settings

c) return to the application list

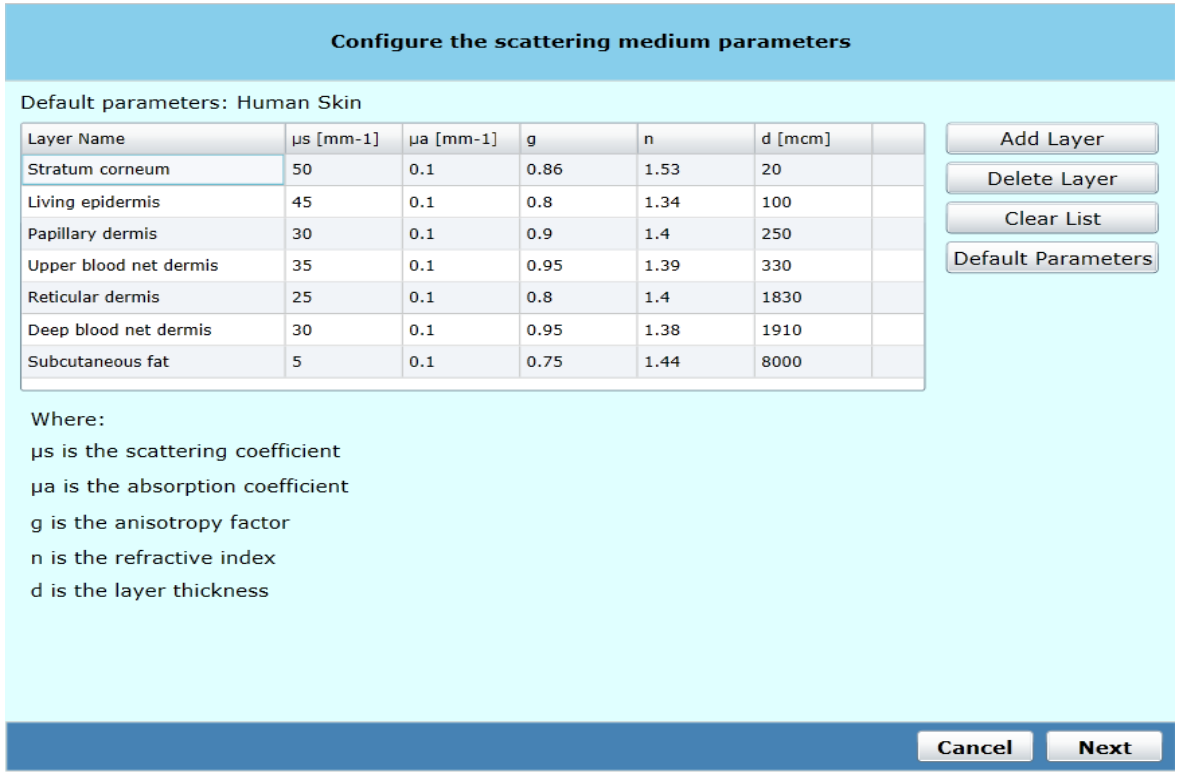




Setting up the parameters of MC

If “Change settings” is clicked than, depending on the chosen application, several dialogs may appear

Scattering medium properties: allows user to add, delete or configure layers of the medium:



If “Cancel” clicked the MC user will return to the application list, “Next” button brings to the further stages of setting up the system (standard and convenient wizard-style application)

Setting up the parameters of MC

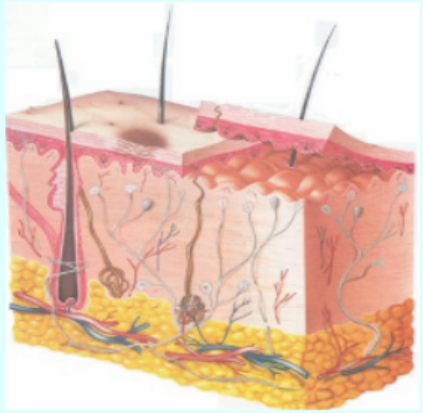
Varying percentage of melanin, blood saturation, hematocrit and water fraction by editing the list in WYSIWYG (what you see is what you get) style

Configure the human skin parameters

Melanin concentration [%]: 2

Default parameters: Human Skin

Layer Name	S blood [%]	Ht [%]	Hm [%]	C water [%]
Stratum corneum	0	0	0	2
Living epidermis	0	0	0	5
Papillary dermis	70	45	18	17
Upper blood net dermis	70	45	19	19
Reticular dermis	75	45	20	16
Deep blood net dermis	75	45	20	17
Subcutaneous fat	75	45	20	11



Default Parameters

Where:

S blood is the oxygen saturation of blood

Ht is the hematocrit index

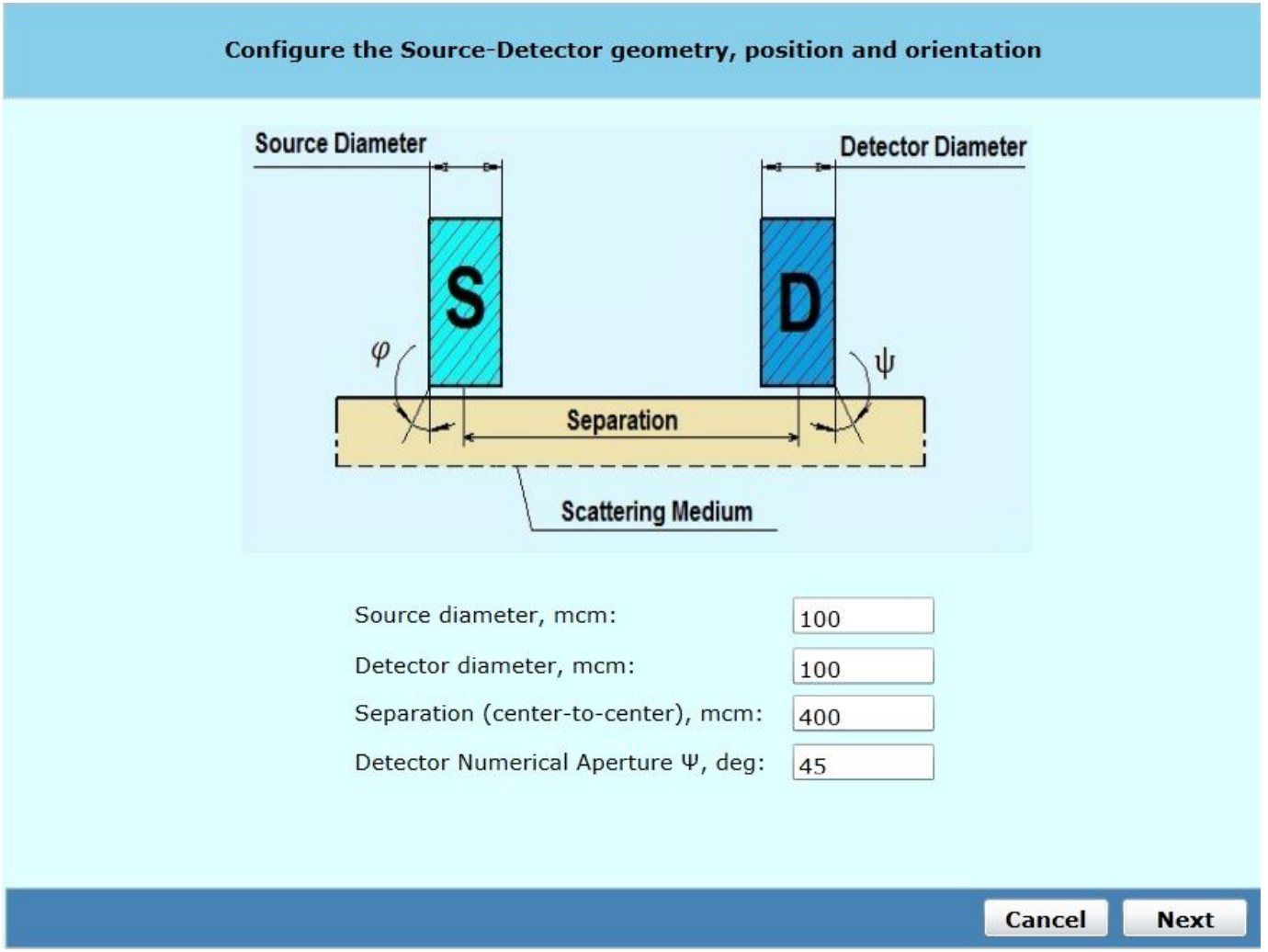
Hm is the hemoglobin fraction

C water is the volume fraction of water

Cancel Next

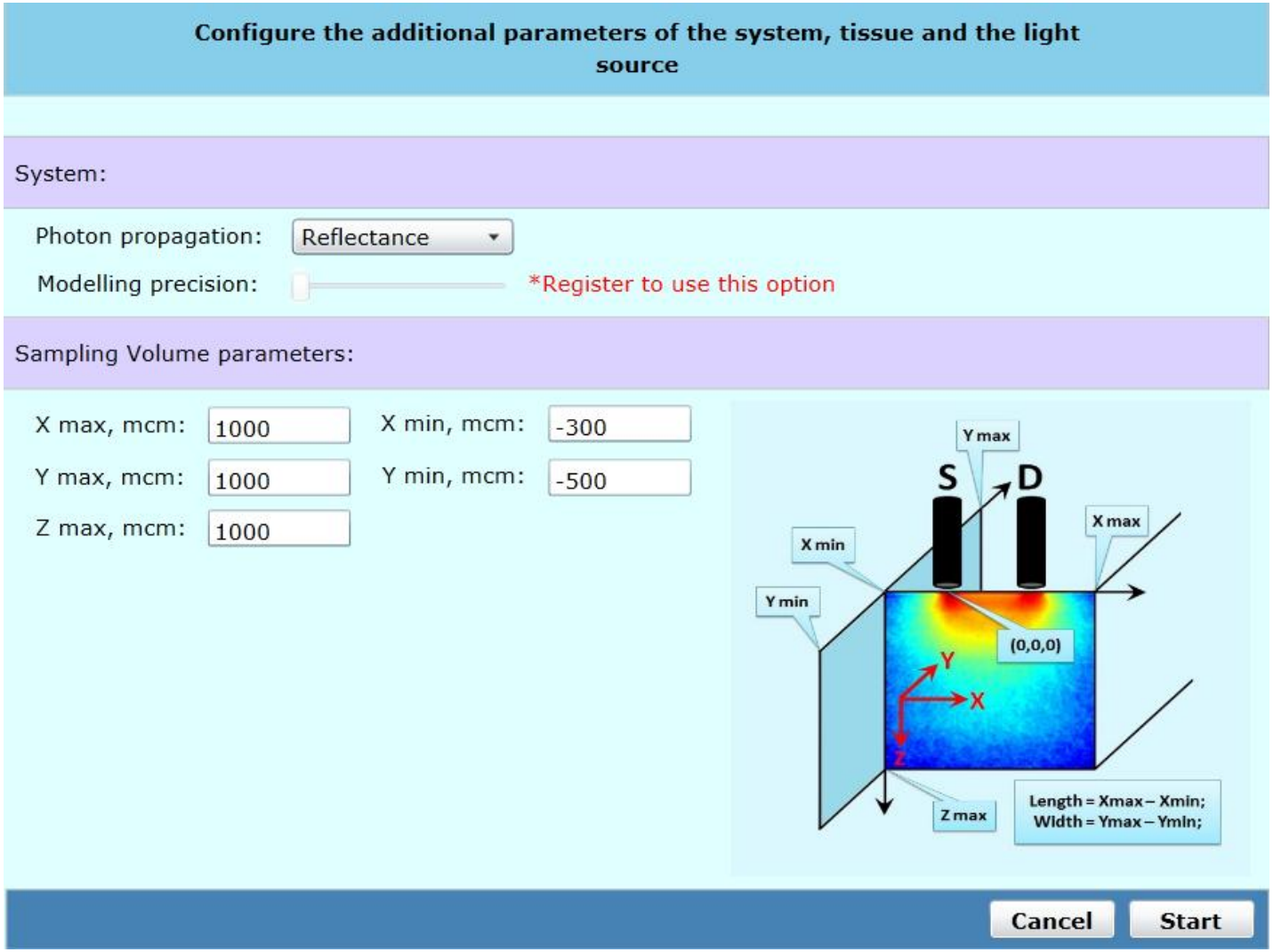
Setting up the parameters of MC

Probe Configuration tab allows setting up the geometry, position, orientation of source and detector used in the MC modelling



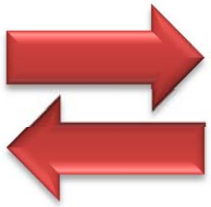
Setting up the parameters of MC

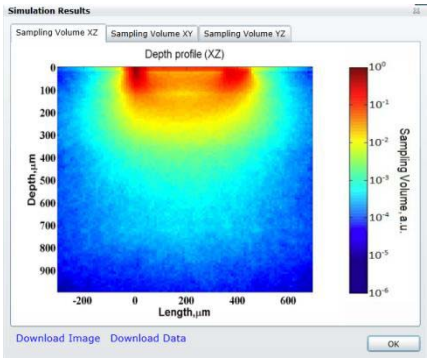
Additional properties allow changing the direction of photon propagation, modelling precision and parameters of the sampling volume distribution.

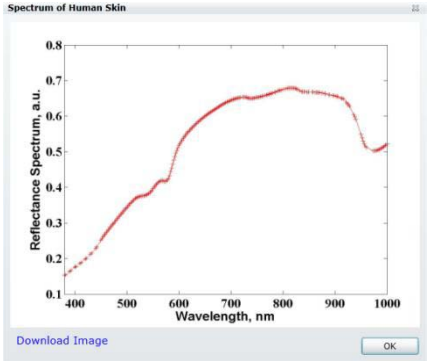


Performing the modeling/ Obtaining results

Our powerful server will perform MC modelling in few seconds, the results will appear in a typical journal paper format.





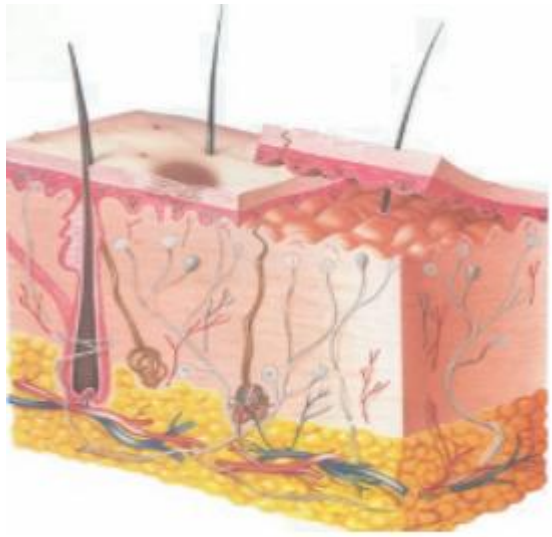


Both results and data can be downloaded and further used in various scientific software packages

Result and Discussion: Modelling of Human Skin Reflectance Spectrum and Colour

The 7-layer-model of human skin used in the GPU-accelerated Object Oriented Monte Carlo model for simulations of human skin spectrum and colour

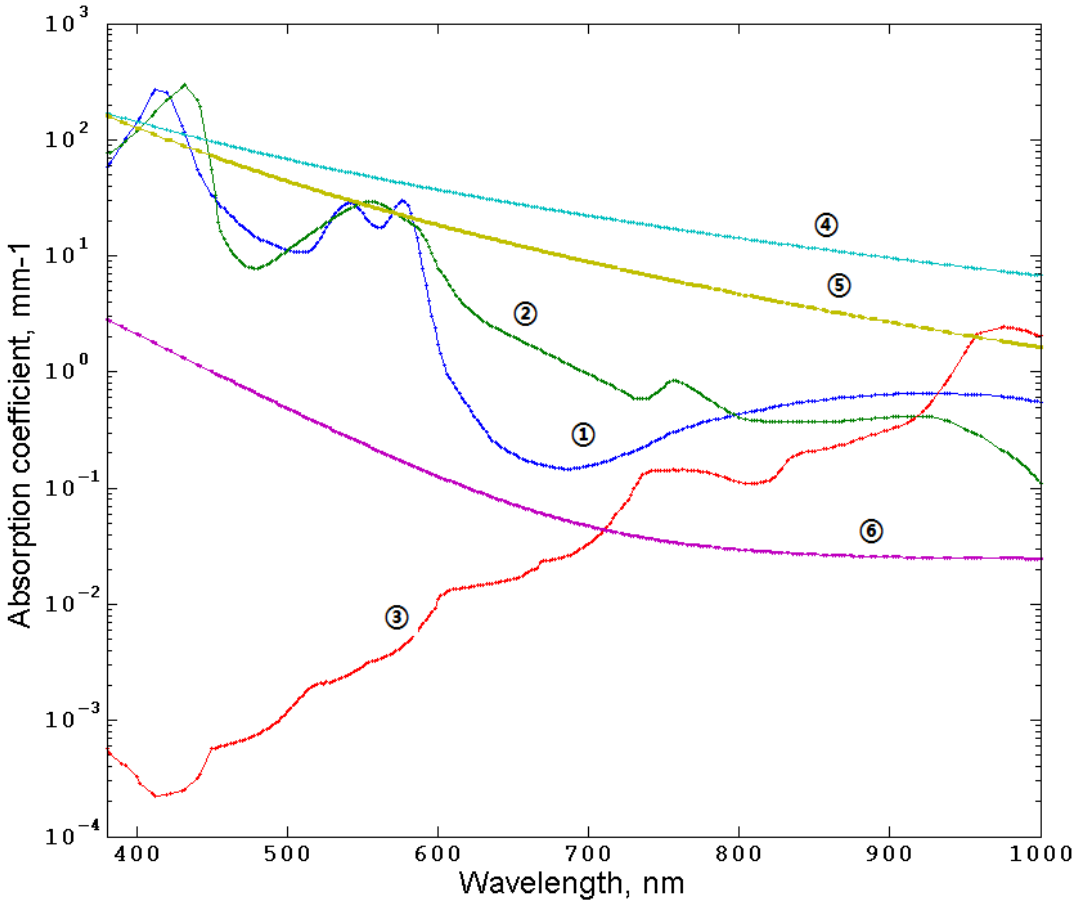
Name of Layer	d	n	C_{blood}	S	Ht	F_{Hb}	F_{RBC}	C_{H20}
Stratum corneum	20	1.53	0	0	0	0		0.02
Living epidermis	150	1.34	0	0	0	0		0.05
Papillary dermis	250	1.4	0.2	0.6	0.4	0.99	0.25	0.2
Upper blood net dermis	330	1.39	0.4	0.7	0.45	0.99	0.25	0.3
Reticular dermis	1830	1.4	0.5	0.75	0.45	0.99	0.25	0.4
Deep blood net dermis	1910	1.38	0.4	0.75	0.5	0.99	0.25	0.4
Subcutaneous fat	8000	1.44	0.05	0.7	0.45	0.99	0.25	0.5



Where: **d** is thickness; **n** is refractive index; $\mathbf{C_{blood}}$ is blood concentration; **S** is blood saturation; **Ht** is hematocrit; $\mathbf{F_{Hb}}$ is volume fraction of haemoglobin in erythrocytes; $\mathbf{F_{RBC}}$ is volume fraction of erythrocytes in the total volume of all blood cells; $\mathbf{C_{H20}}$ is water concentration, respectively

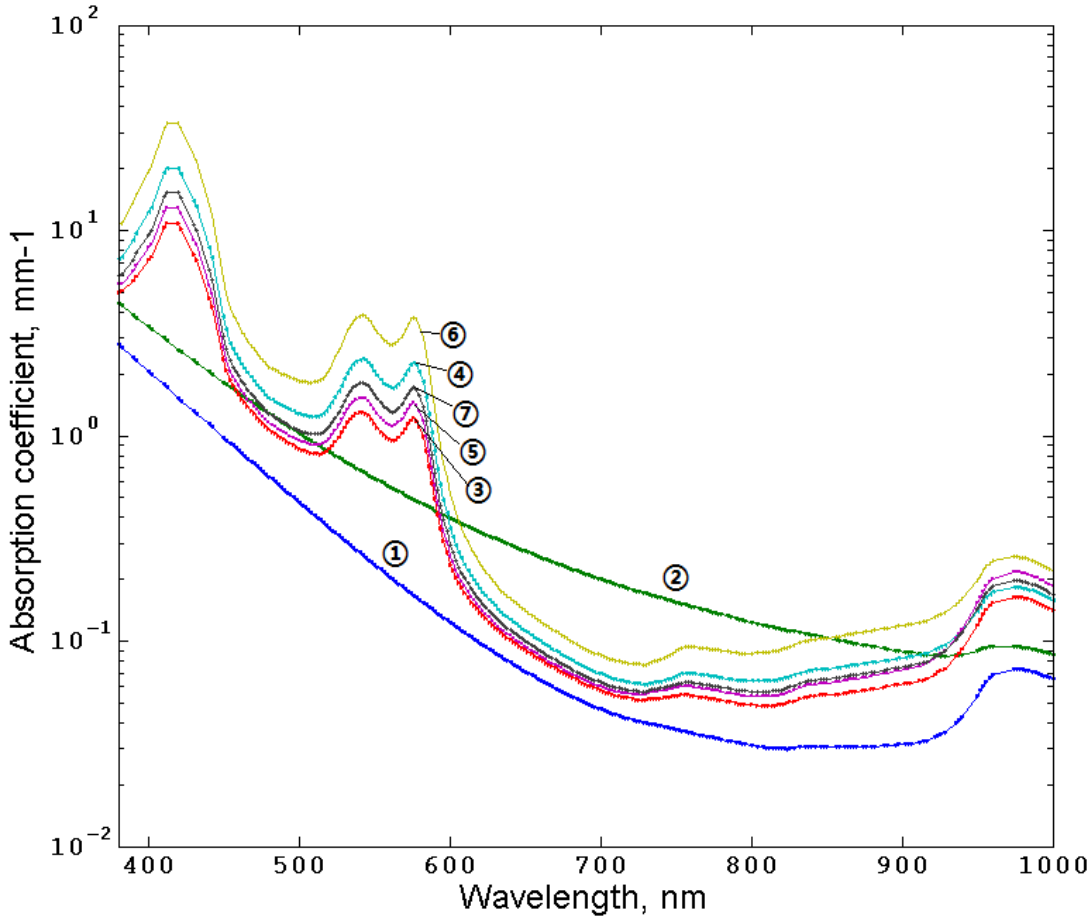
- **Scattering, absorption and anisotropy factor vary over the wavelength range from 380 to 1000 nanometres during the MC simulation**
- **Melanin fraction, melanin blend and haemoglobin fraction vary during the simulation from 0-45% ,0-100%,0-75% respectively**

Human Skin Optics: Some key components



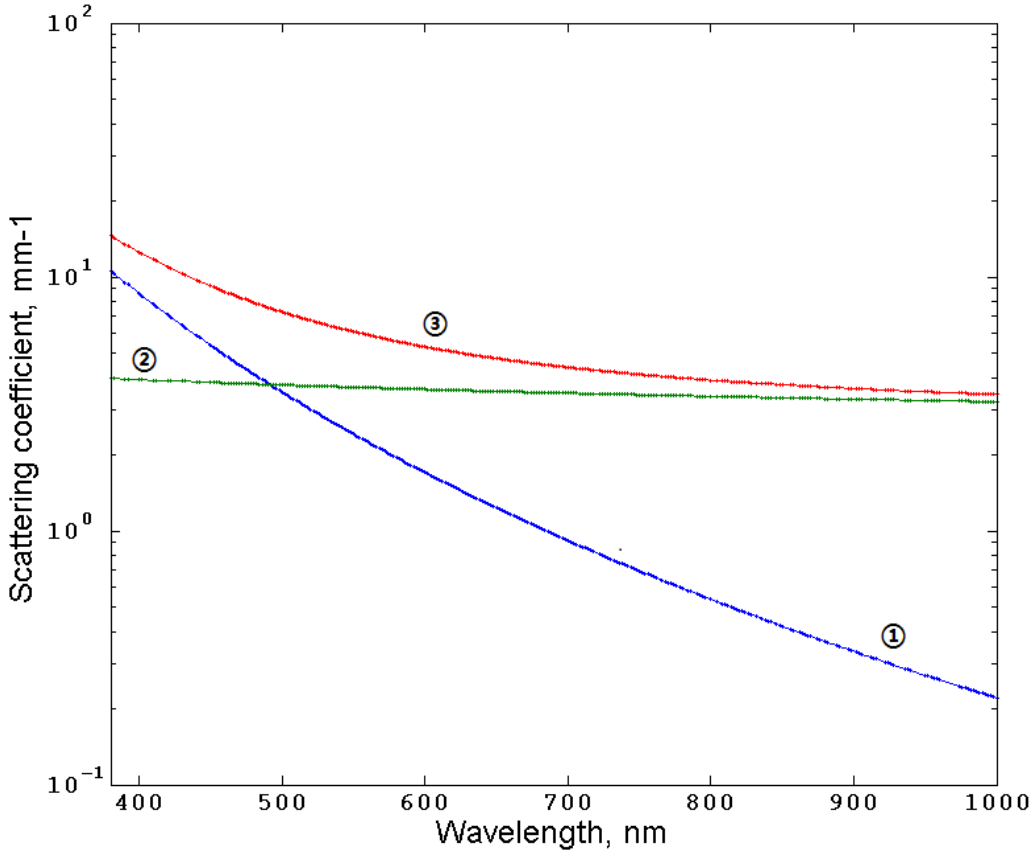
Schematic presentation of some key absorption coefficients where: 1 – HB02, 2 - HB, 3 - Water, 4 - Eumelanin, 5 - Pheomelanin, 6 - Baseline

Human Skin Optics: Absorption



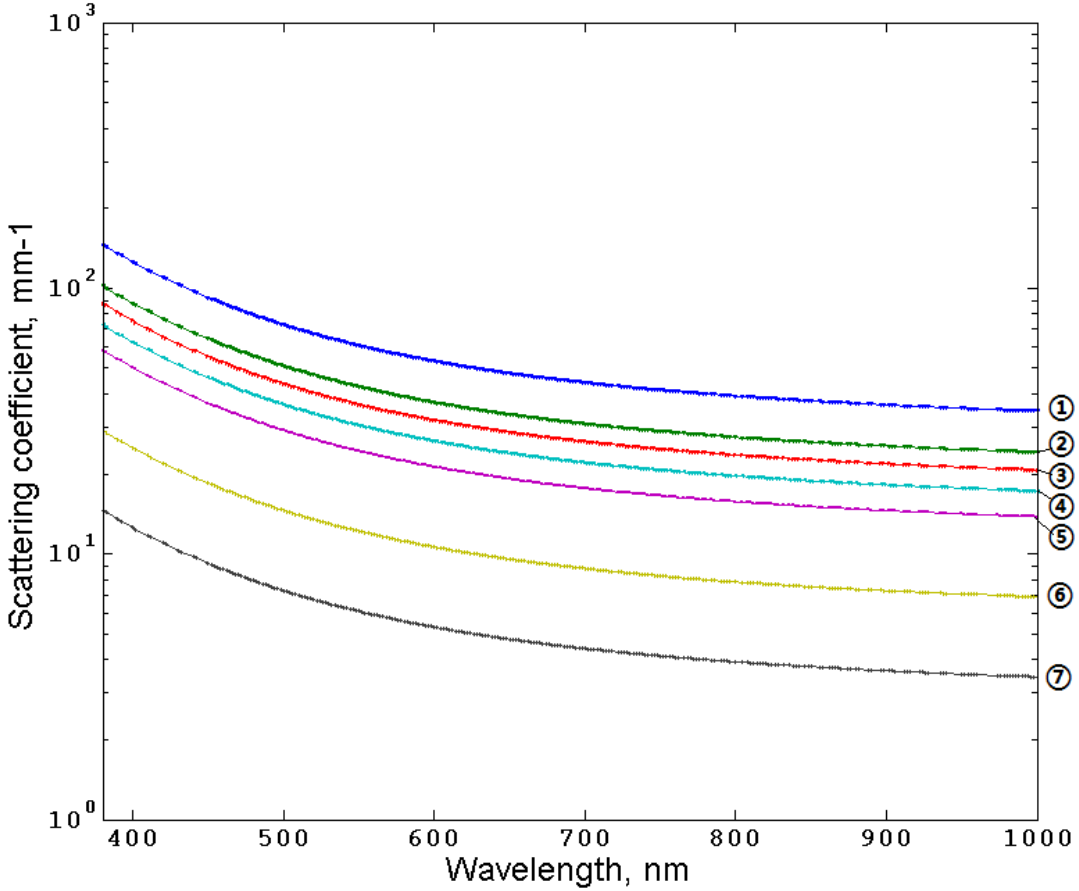
Schematic presentation of human skin absorption coefficients where: 1 - Stratum Corneum, 2 - Living Epidermis, 3 - Papillary Dermis, 4 - Upper Blood Net Dermis, 5 - Reticular Dermis, 6 - Deep Blood Net Dermis,7 - Subcutaneous Fat

Human Skin Optics: Scattering



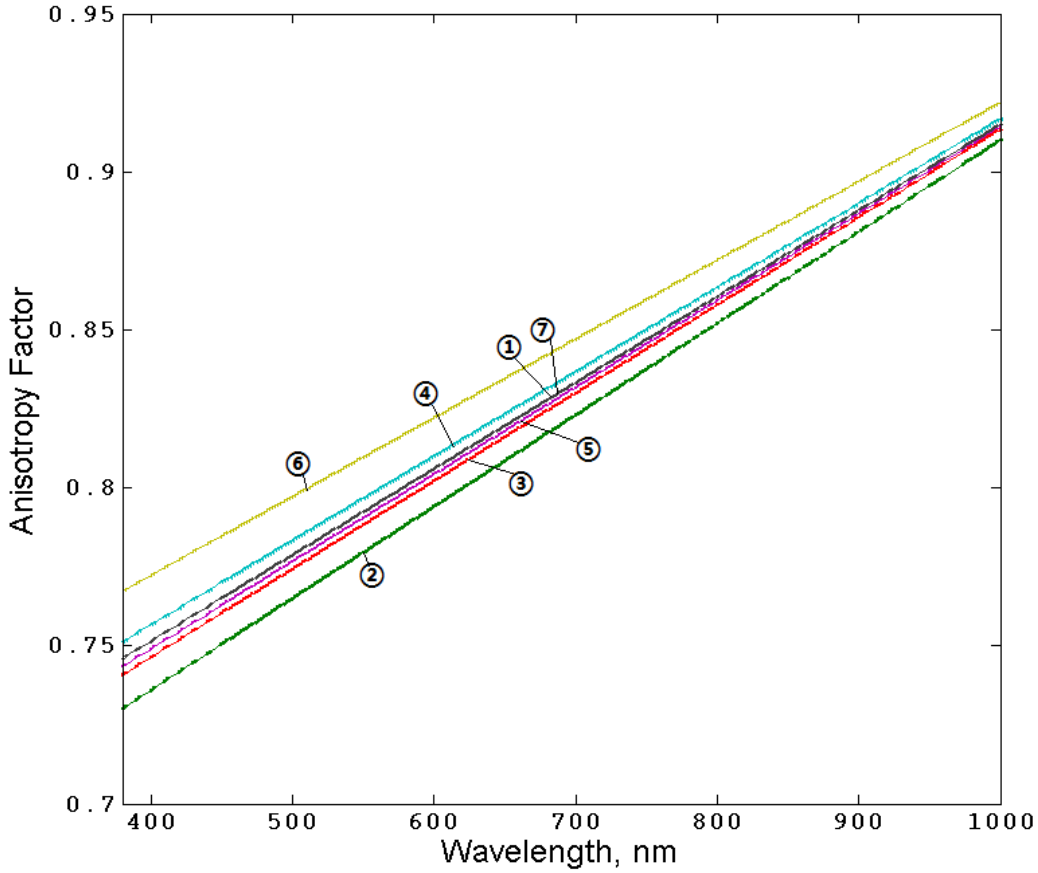
Schematic presentation of some scattering coefficients, including: 1 – Rayleigh, 2 – Mie, 3 – Human skin (reduced)

Human Skin Optics: Scattering



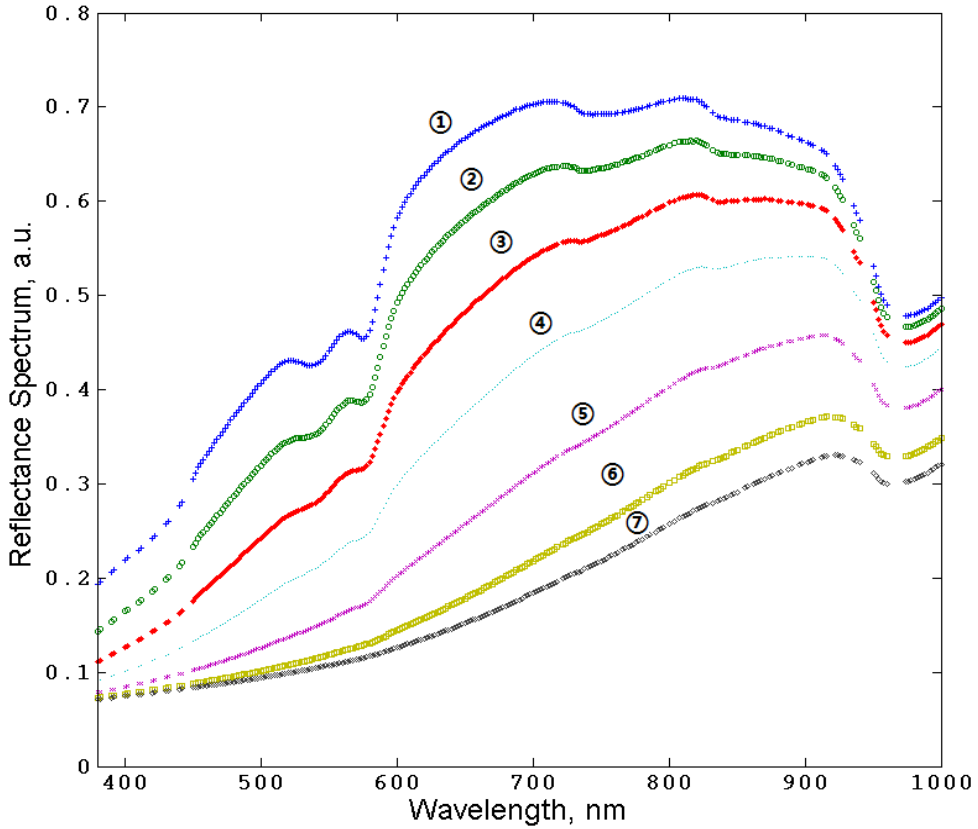
Schematic presentation of human skin scattering coefficients where: 1 - Stratum Corneum, 2 - Living Epidermis, 3 - Papillary Dermis, 4 - Upper Blood Net Dermis, 5 - Reticular Dermis, 6 - Deep Blood Net Dermis,7 - Subcutaneous Fat

Human Skin Optics: Anysotropy



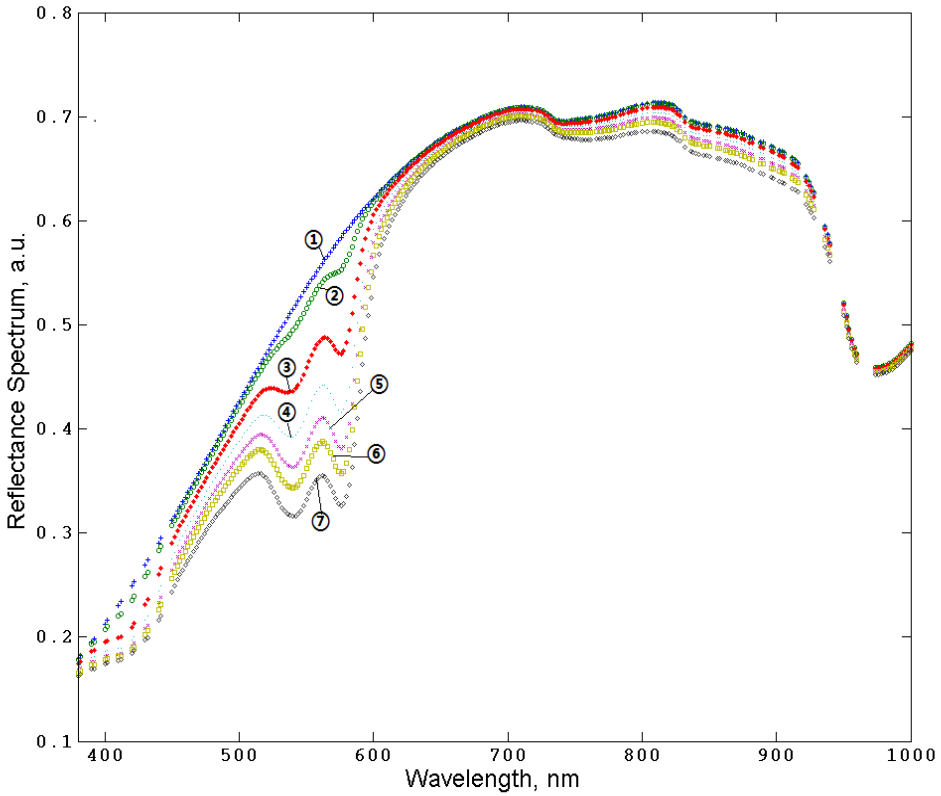
Schematic presentation of human anisotropy factor where: 1 - Stratum Corneum, 2 - Living Epidermis, 3 - Papillary Dermis, 4 - Upper Blood Net Dermis, 5 - Reticular Dermis, 6 - Deep Blood Net Dermis,7 - Subcutaneous Fat

Results: simulating human skin reflectance spectrum and colour



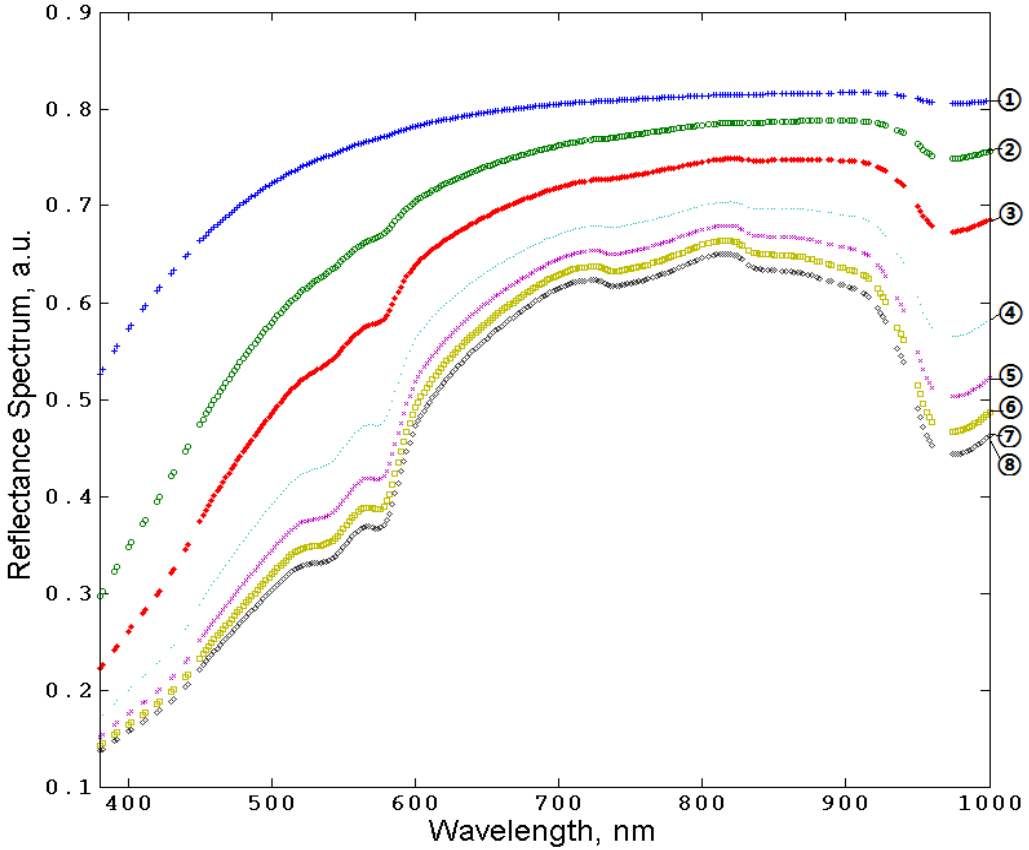
Varying the melanin fraction: (1)-0%, (2)-2%, (3)-5%,(4)-10%, (5)-20%,(6)-35%,(7)-45%, respectively; the blend between eumelanin and pheomelanin is 1:3

Results: simulating human skin reflectance spectrum and colour



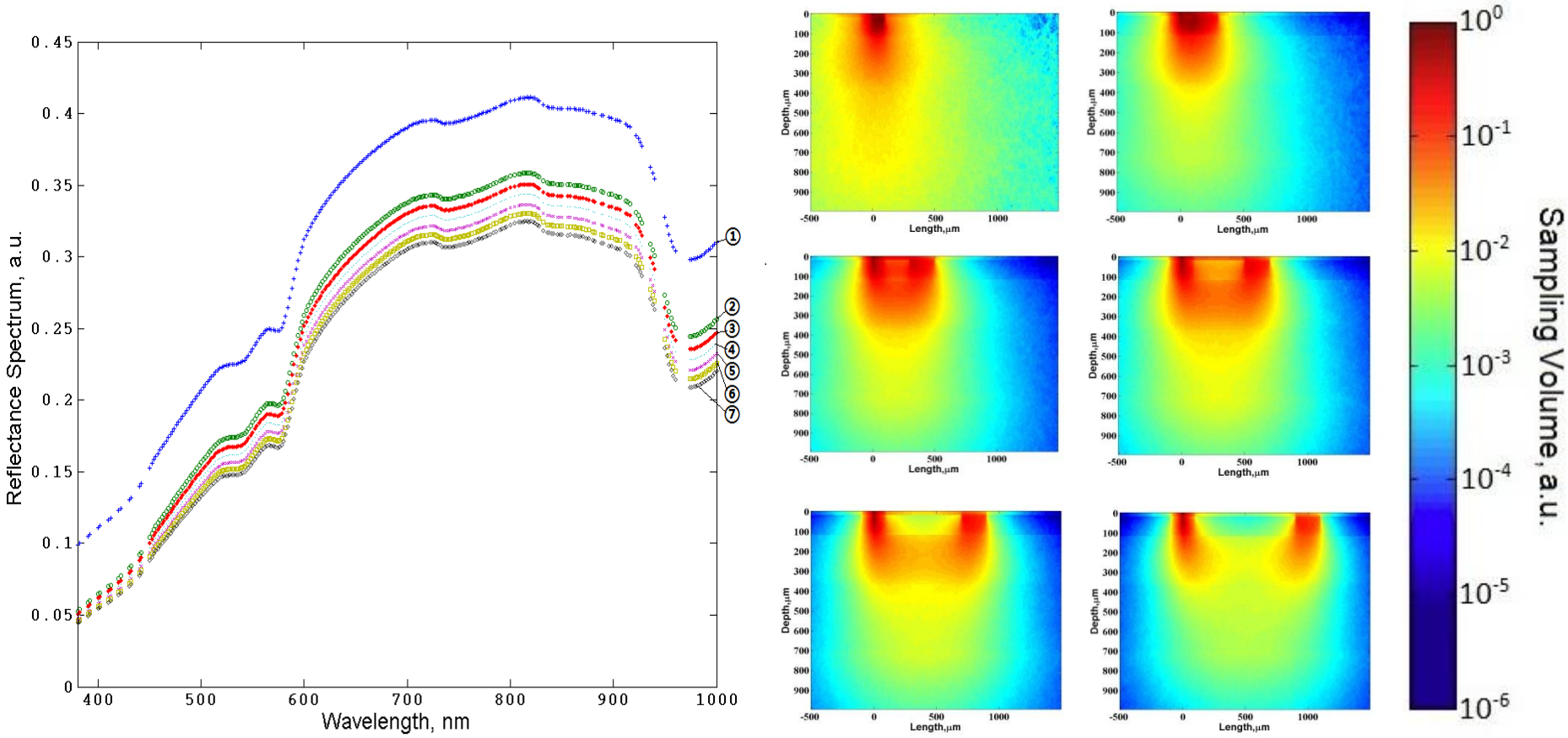
Varying the haemoglobin fraction in the layers from papillary dermis to subcutaneous tissue: (1)-0%, (2)-2%, (3)-5%,(4)-10%, (5)-20%,(6)-35%,(7)-70%, respectively; melanin fraction is 0%; blend between eumelanin and pheomelanin is 1:3;

Results: varying detector diameter



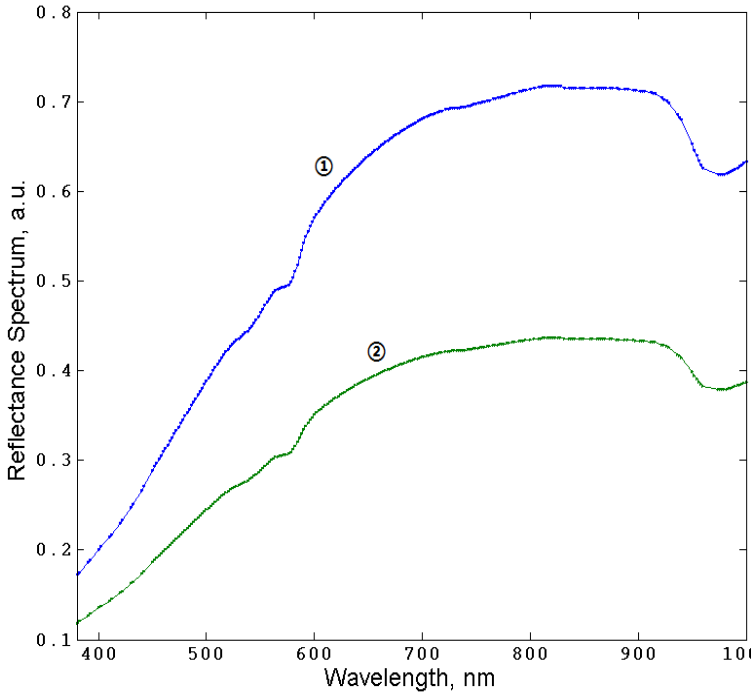
Varying detector's (integral sphere) diameter: (1)-100 mcm, (2)-300mcm, (3)-500 mcm, (4)-1000 mcm, (5)-2000 mcm, (6)-3000 mcm, (7)-5000 mcm, (8)-10000 mcm, respectively

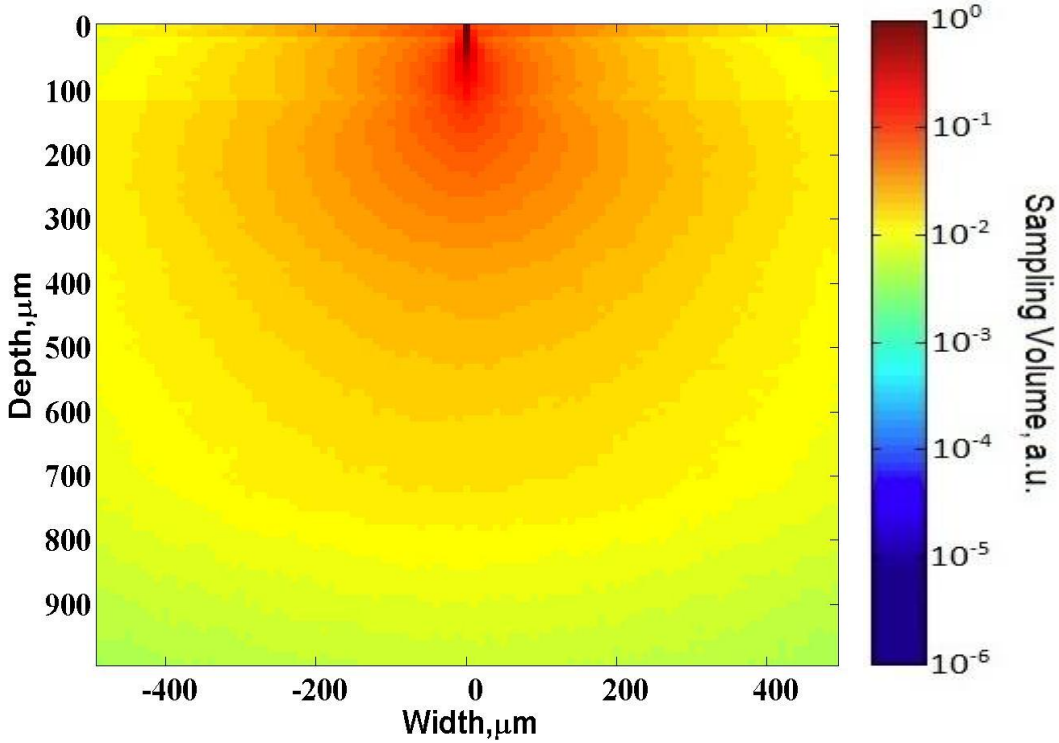
Results: varying source-detector separation



Varying the separation between source (Ø200mcm) and detector (Ø200mcm) detector's (integral sphere) diameter: (1)-0 mcm, (2)-200mcm, (3)-300 mcm, (4)-400 mcm, (5)-600 mcm, (6)-800mcm, (7)-1000mcm, respectively; detector's numerical aperture is 20°

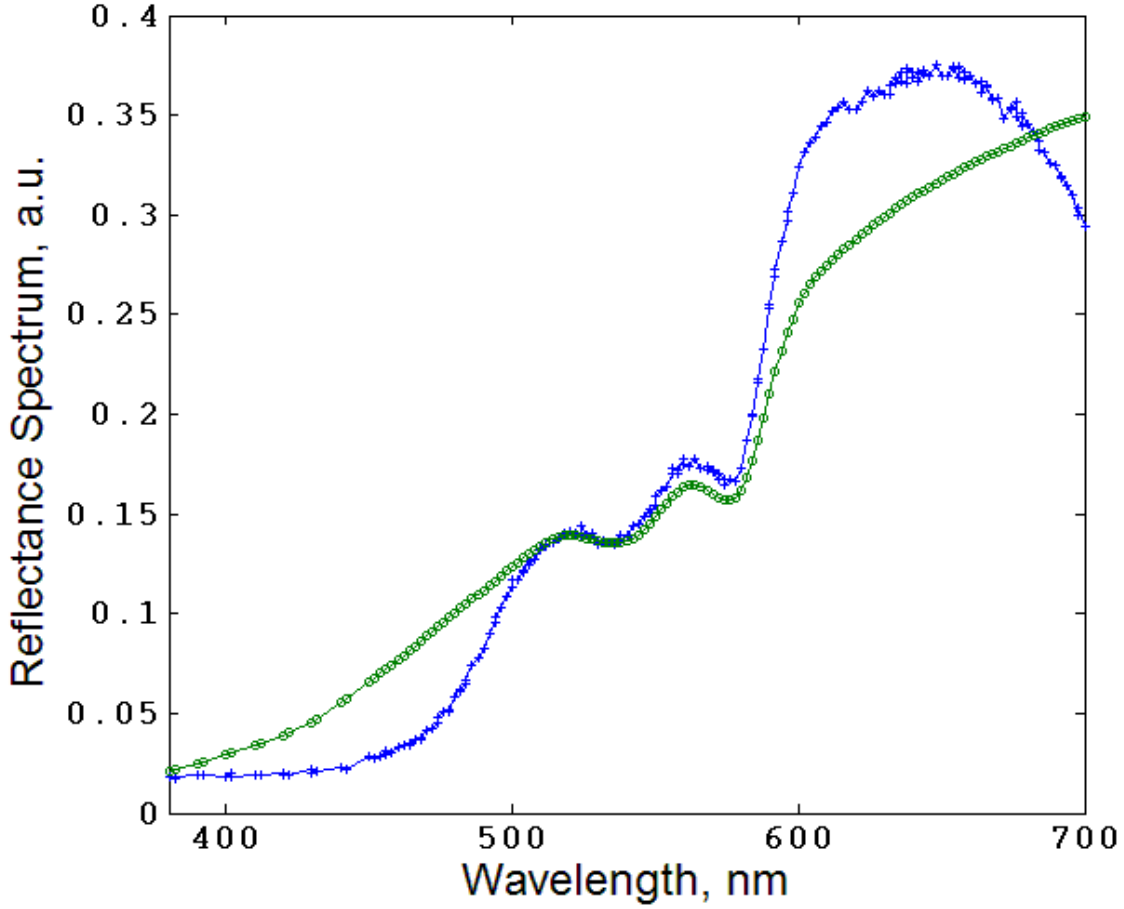
Results: towards spectrum modelling

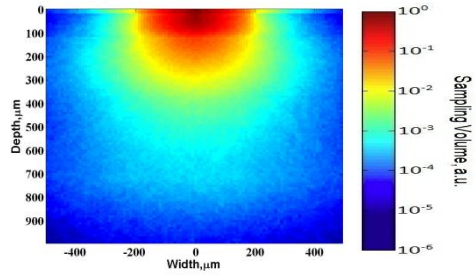




Employing two different approaches while modelling spectrum of human skin (integral sphere configuration): (1) using the number of photons detected one time as a factor; (2) utilizing the total diffuse reflectance Rd technique

Results: comparison with measured in vivo





Schematic presentation of the reflectance spectrum measured in vivo (1) using an Ocean Optics USB4000 spectrometer, probe QR400-7-VIS-NIR (SD=DD=XD=400mcm, NA = 24.8) with modelling (2), employing the developed MC technique


TO BE
CONTINUED
WHEN WE
FIND A BETTER
SCRIPT
Parker.

Acknowledgements

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