Generalized diffusion models for transport in scattering and non-scattering regions

Guillaume Bal

Department of Applied Physics & Applied Mathematics

Columbia University

http://www.columbia.edu/∼gb2030

gb2030@columbia.edu

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

Mathematical Problems in Optical Tomography

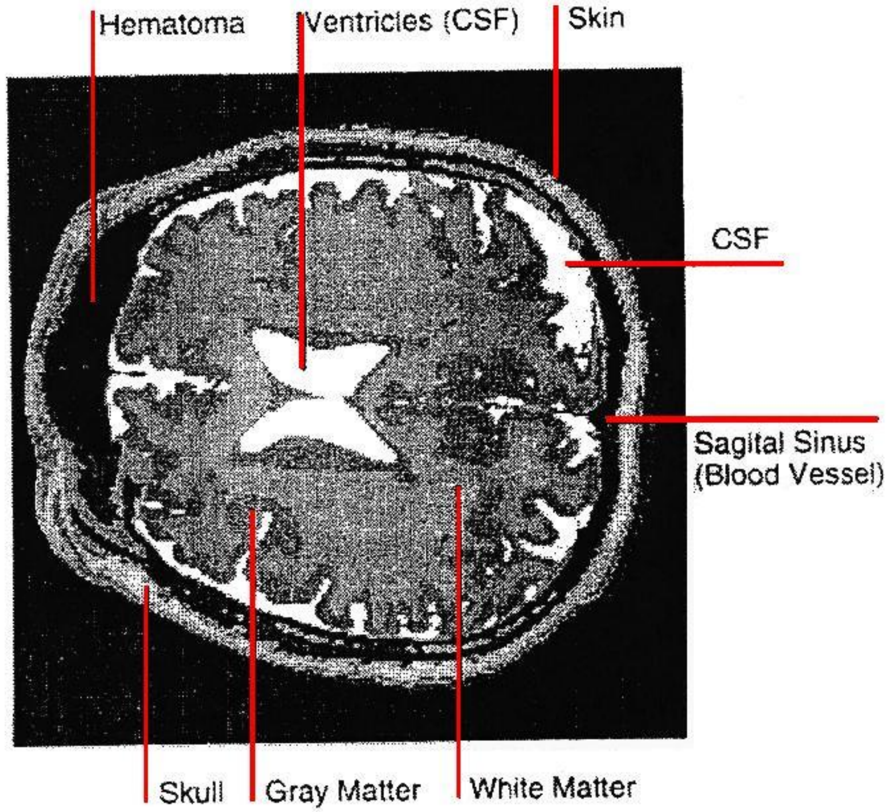
Optical Tomography consists in reconstructing absorption and scattering properties of human tissues by probing them with Near-Infra-Red photons (wavelength of order 1μm; mean free path of order $1-10$mm).

What needs to be done:

- Modeling of forward problem using equations that are easy to solve: photons strongly interact with underlying tissues.

- Devising reconstruction algorithms to image tissue properties from boundary measurements of photon intensities.

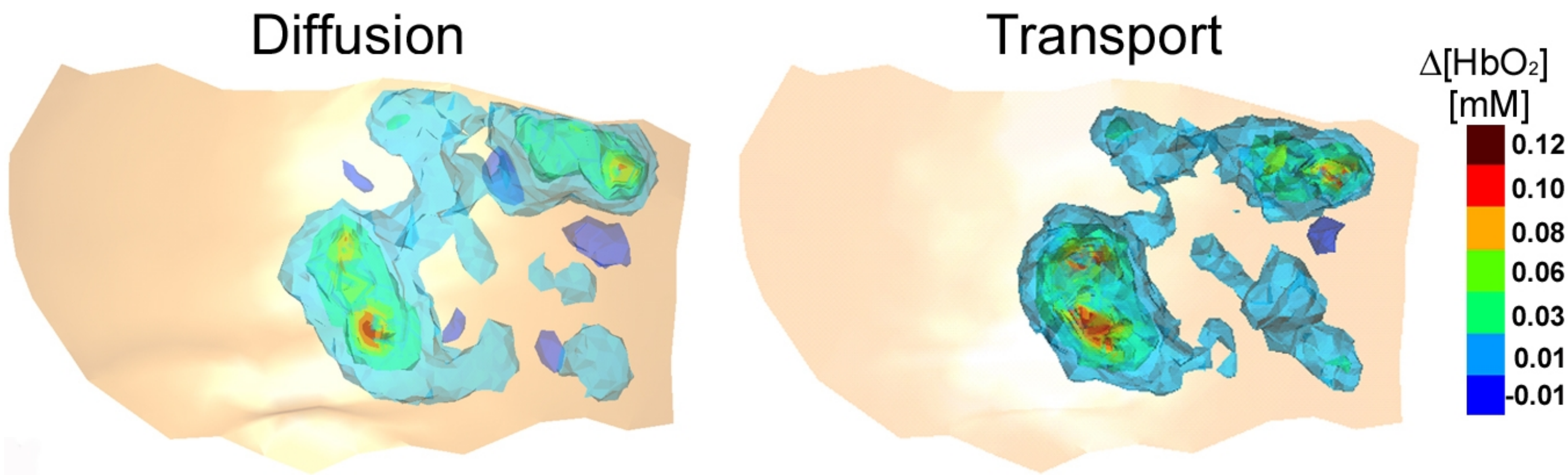
Applications in Near-Infra-Red Spectroscopy



Segmented MRI data for a human brain.

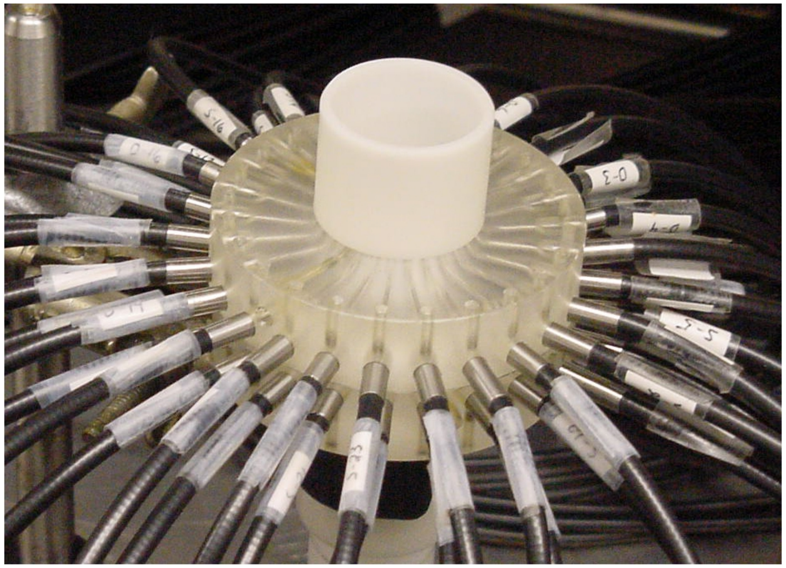
Imaging of human brains.

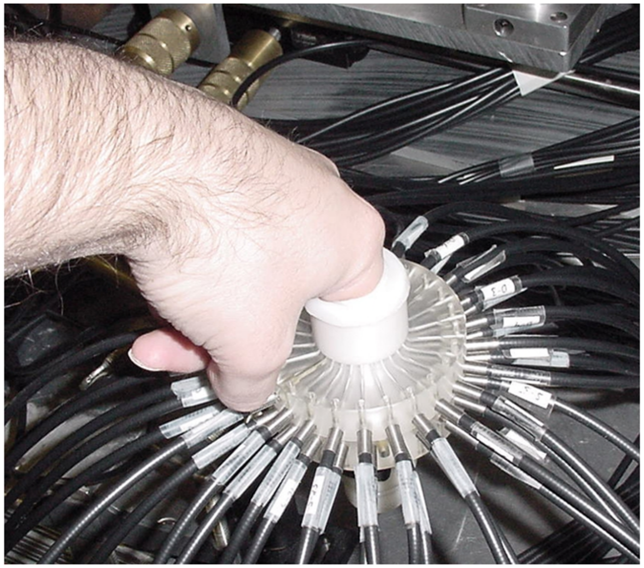
Applications in Near-Infra-Red Spectroscopy



Imaging of human brains (from A.H. Hielscher, biomedical Engineering, Columbia).

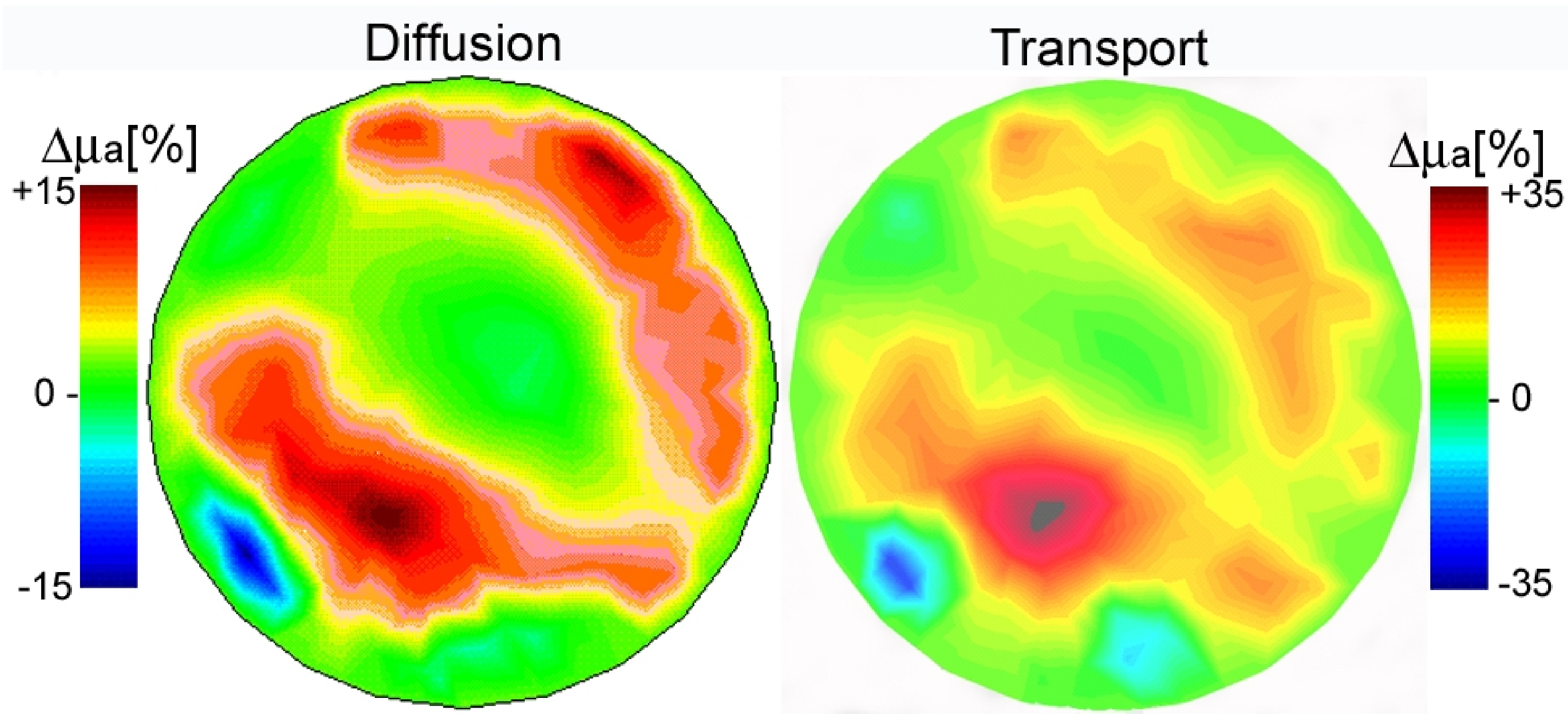
Applications in Near-Infra-Red Spectroscopy





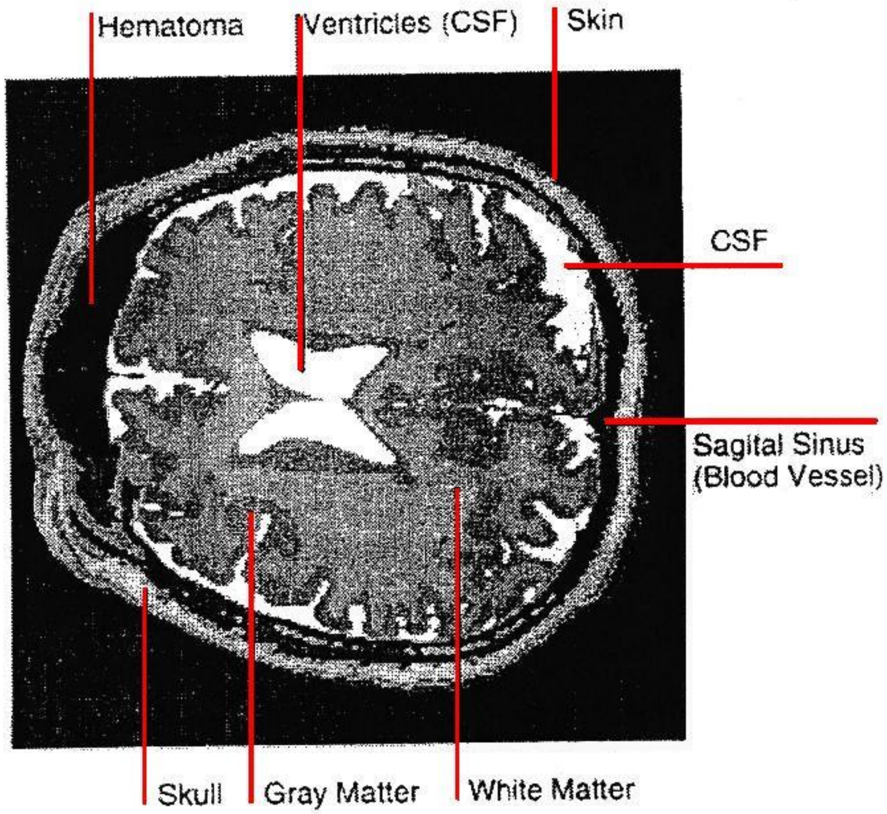
Detection of arthritis in finger joints.

Applications in Near-Infra-Red Spectroscopy



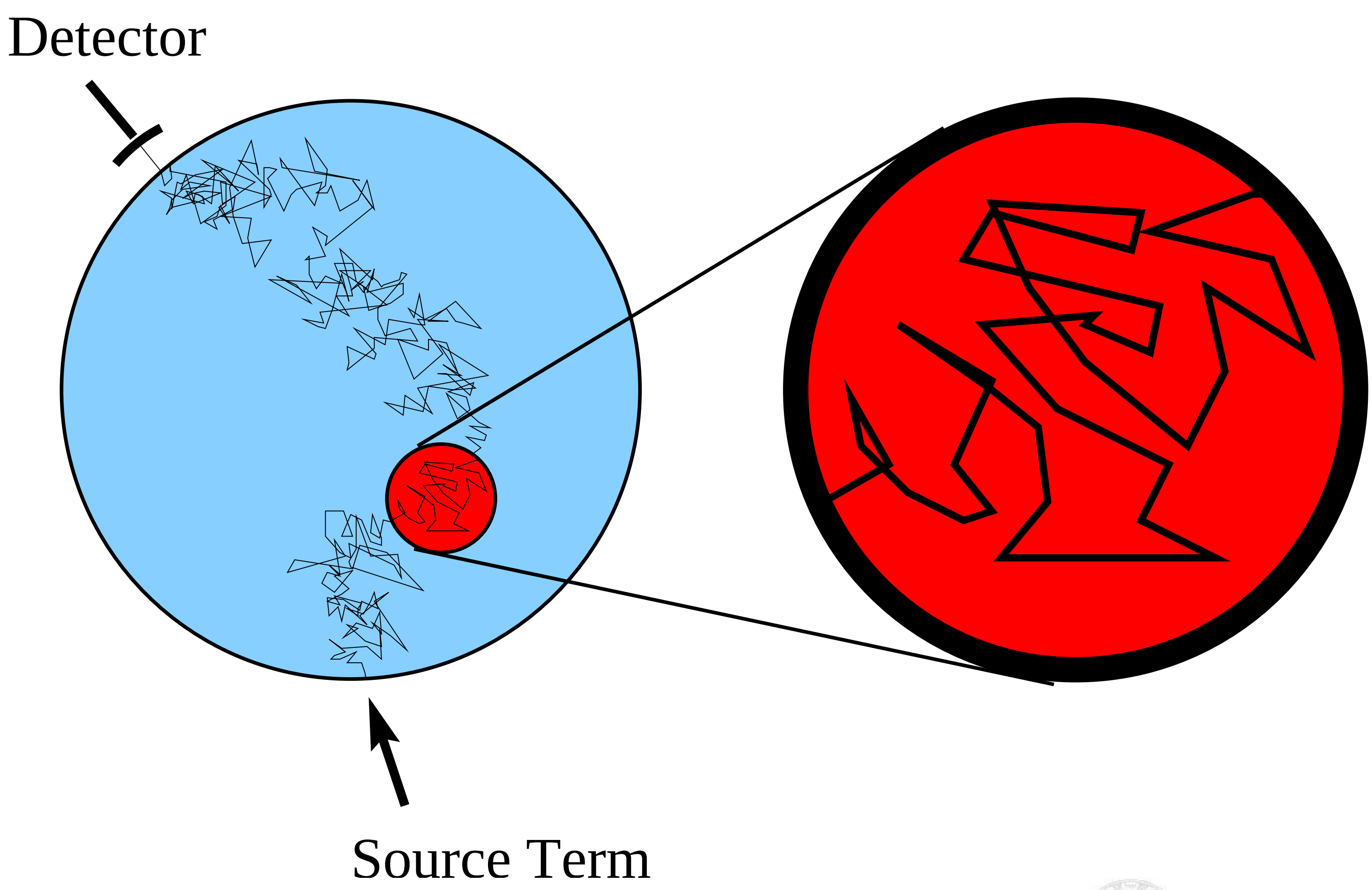
Reconstructed Finger Absorption using different forward models.

An example of modeling difficulty: Clear layers embedded in scattering tissues

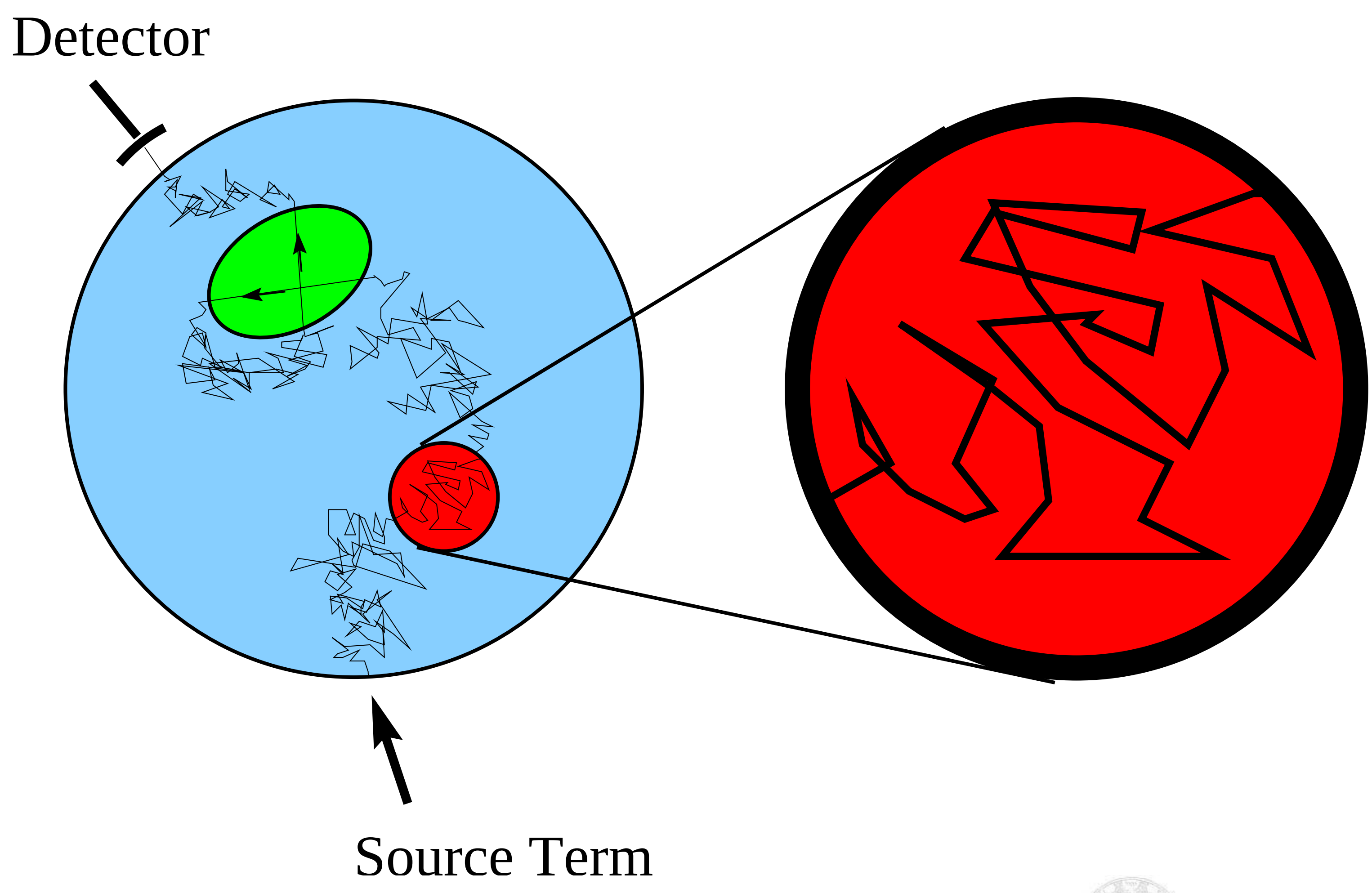


Segmented MRI data for a human brain.

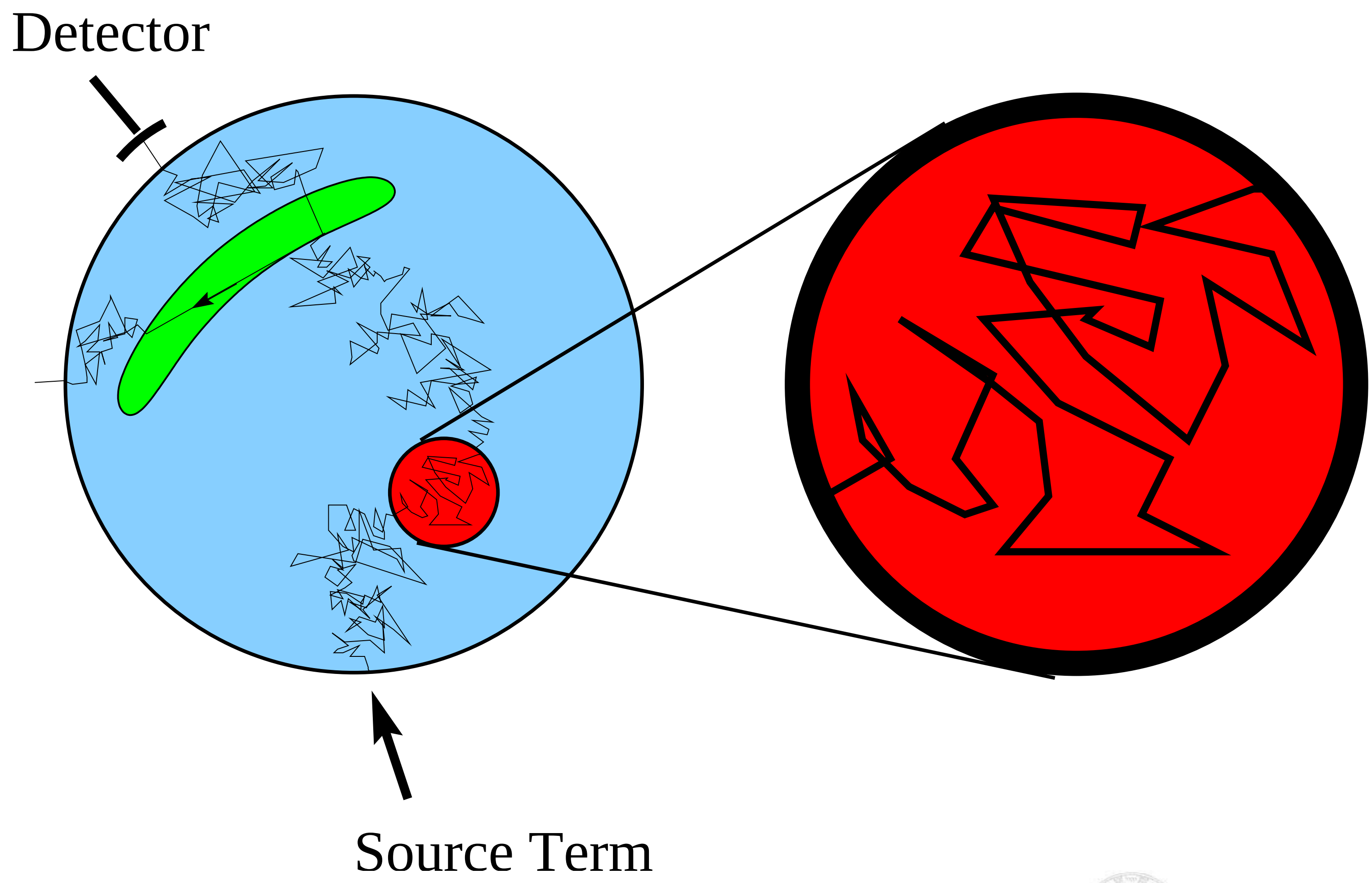
Typical path of a detected photon in a DIFFUSIVE REGION



Same typical path in the presence of a CLEAR INCLUSION



Same typical path in the presence of a CLEAR LAYER



Modeling of Forward Problem:

To derive macroscopic equations that model photon propagation *both* in the diffusive and non-diffusive domains.

Outline:

1. Brief recall on the derivation of diffusion equations
2. Modified equations in the presence of Embedded Objects
3. Generalized equations in the presence of Clear Layers
4. Numerical simulation of transport and diffusion models

Transport Equation and Scaling

The phase-space linear transport equation is given by

$$\begin{aligned} &\frac{1}{\varepsilon} v \cdot \nabla u_\varepsilon(x,v) + \frac{1}{\varepsilon^2} Q(u_\varepsilon)(x,v) + \sigma_a(x) u_\varepsilon(x,v) = 0 \qquad \text{in } \Omega \times V, \\ &u_\varepsilon(x,v) = g(x,v) \qquad \text{on } \Gamma_- = \{(x,v) \in \partial\Omega \times V \text{ s.t. } v \cdot \nu(x) < 0\}. \end{aligned}$$

$u_\varepsilon(x,v)$ is the particle density at $x \in \Omega \subset \mathbb{R}^3$ with direction $v \in V = S^2$.
The scattering operator Q is defined by

$$Q(u)(x,v) = \sigma_s(x)\Big(u(x,v) - \int_V u(x,v') d\mu(v') \Big).$$

The mean free path ε measures the mean distance between successive interactions of the particles with the background medium.
The diffusion limit occurs when $\varepsilon \to 0$.

Volume Diffusion Equation

Asymptotic Expansion: $u_\varepsilon(x,v) = u_0(x) + \varepsilon u_1(x,v) + \varepsilon^2 u_2(x,v) \ldots$

Equating like powers of ε in the transport equation yields

$$\begin{aligned} \text{Order } \varepsilon^{-2}: \quad & Q(u_0) &=& \; 0 \\ \text{Order } \varepsilon^{-1}: \quad & v\cdot\nabla u_0 + Q(u_1) &=& \; 0 \\ \text{Order } \varepsilon^{0}: \quad & v\cdot\nabla u_1 + Q(u_2) + \sigma_a u_0 &=& \; 0. \end{aligned}$$

Krein-Rutman theory:

$$\text{Order } \varepsilon^{-2}: \quad u_0(x,v) = u_0(x)$$

$$\text{Order } \varepsilon^{-1}: \quad u_1(x,v) = -\frac{1}{\sigma_s(x)} v\cdot\nabla u_0(x),$$

$$\text{Order } \varepsilon^{0}: \quad \boxed{-\text{div} D(x)\cdot\nabla u_0(x) + \sigma_a(x) u_0(x) = 0 \qquad \text{in } \Omega}$$

where the diffusion coefficient is given by $\boxed{D(x) = \dfrac{1}{3\sigma_s(x)}}$

Diffusion Equations with Boundary Conditions

The volume asymptotic expansion does not hold in the vicinity of boundaries. After boundary layer analysis we obtain

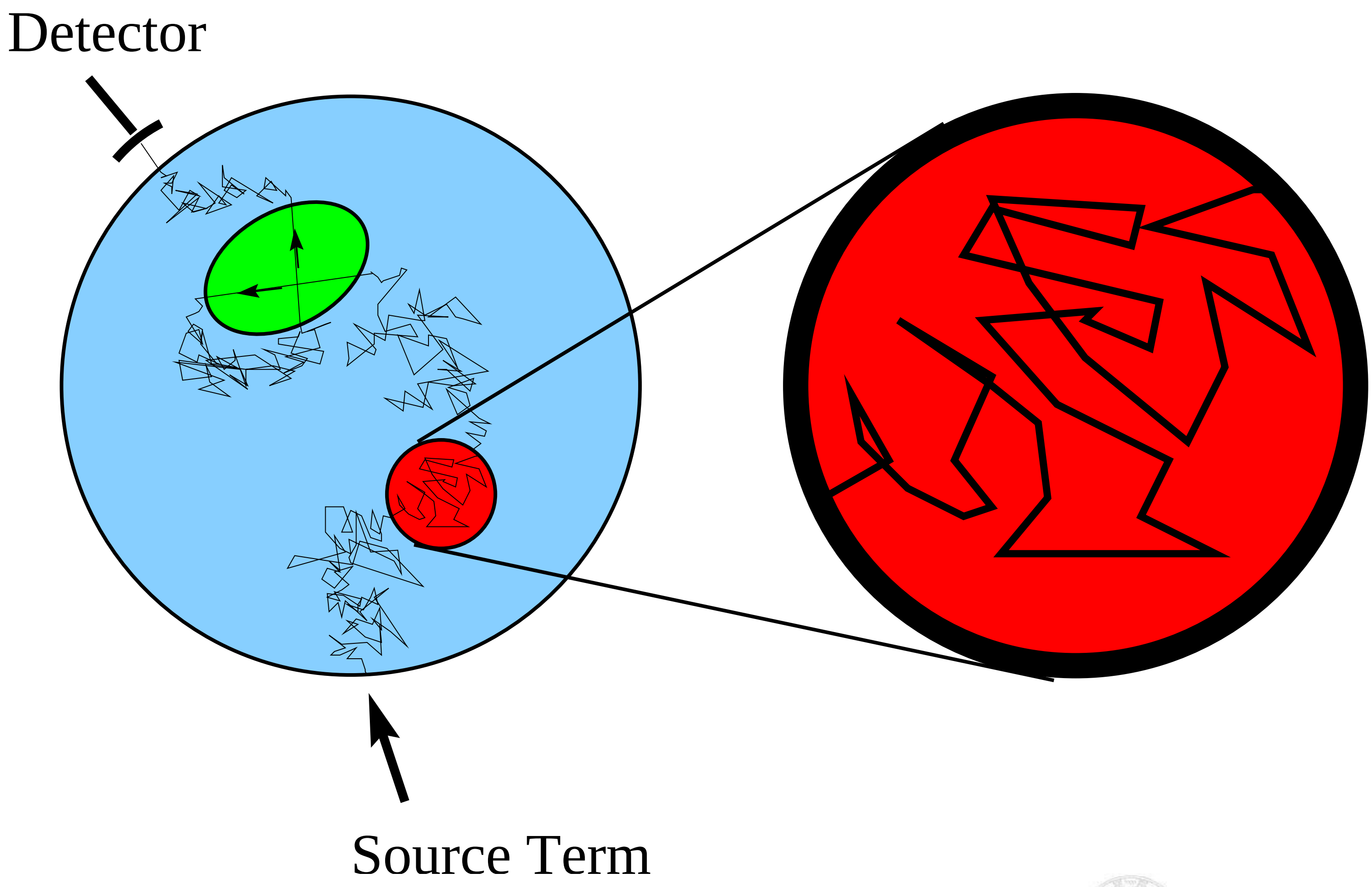
$$-\text{div} D(x) \cdot \nabla u_0(x) + \sigma_a(x) u_0(x) = 0 \quad \text{in} \quad \Omega$$
$$u_0(x) = \Lambda(g(x,v)) \qquad \text{on} \quad \partial\Omega.$$

Λ is a linear form on $L^\infty(V_-)$.

We obtain in any reasonable sense that

$$\boxed{u_\varepsilon(x,v) = u_0(x) + O(\varepsilon).}$$

Generalization to the case of a Clear Embedded Object of size $O(1)$



Diffusion Equation with Non-Local equilibrium

Let Ω^C be the Clear Inclusion and $\Omega^E = \Omega \backslash \Omega^C$. The transport equation is

$$\begin{aligned}
&\frac{1}{\varepsilon} v \cdot \nabla u_\varepsilon(x,v) + \frac{1}{\varepsilon^2} Q(u_\varepsilon)(x,v) + \sigma_a(x) u_\varepsilon(x,v) = 0 && \text{in } \Omega^E \times V \\
&u_\varepsilon(x,v) = g(x,v) && \text{on } \Gamma_- \\
&v \cdot \nabla u_\varepsilon^c(x,v) + Q^c(u_\varepsilon^c)(x,v) + \varepsilon \sigma_{a1} u_\varepsilon^c(x,v) = 0 && \text{in } \Omega^C \times V \\
&u_\varepsilon(x,v) = u_\varepsilon^c(x,v) && \text{on } \partial\Omega^C \times V.
\end{aligned}$$

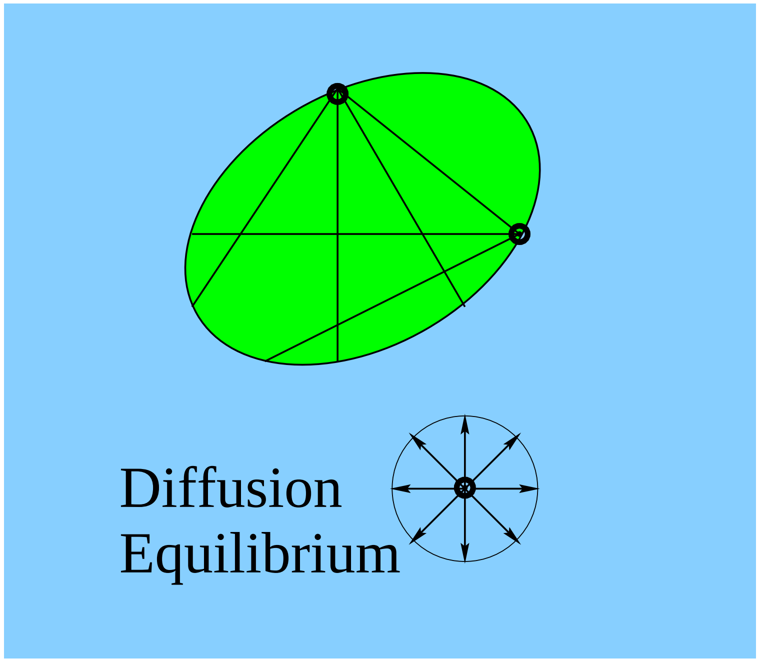
The solution $u_\varepsilon(x,v)$ converges to $u_0(x)$ strongly in $L^2(\Omega^E \times V)$, where

$$\begin{aligned}
&-\text{div} D(x) \cdot \nabla u_0(x) + \sigma_a(x) u_0(x) = 0 && \text{in } \Omega^E \\
&u_0(x) = \Lambda(g(x,v)) && \text{on } \partial\Omega,
\end{aligned}$$

and

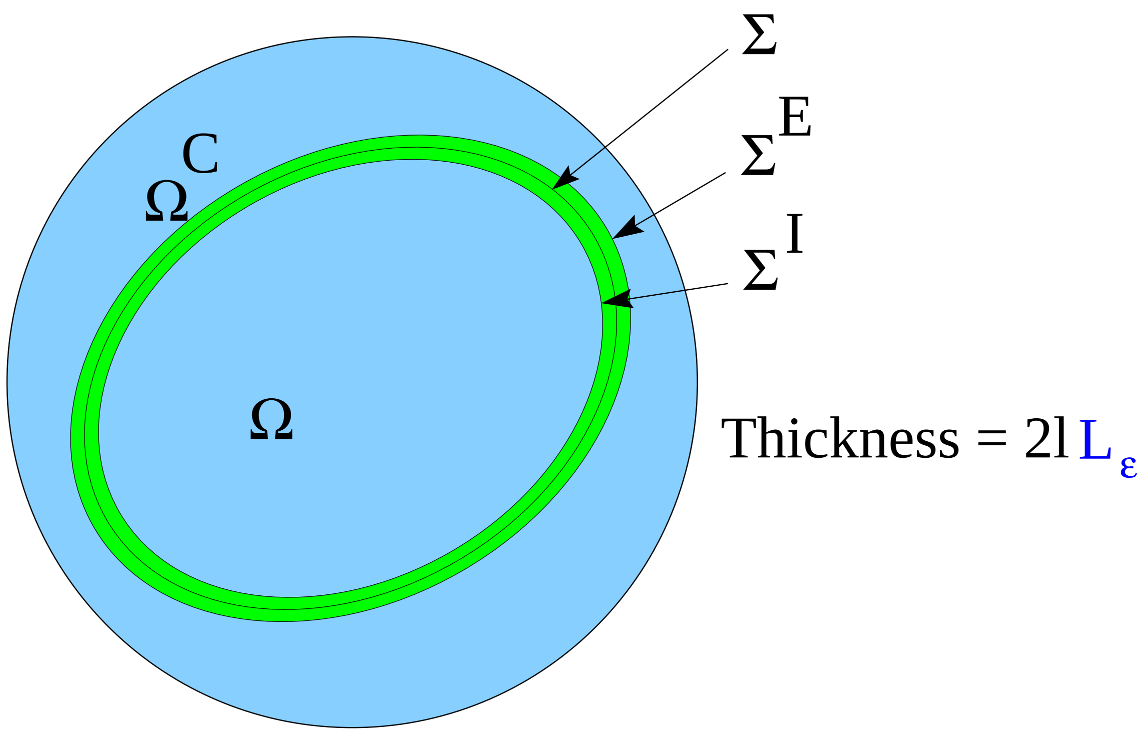
$$\boxed{\begin{aligned}
&u_0(x) = \text{Constant} \qquad \text{on } \partial\Omega^C \\
&\int_{\partial\Omega^C} D(x) \nu^E \cdot \nabla u_0 \, d\sigma(x) + u_{0|\partial\Omega^C} \int_{\Omega^C} \sigma_{a1}(y) dy = 0.
\end{aligned}}$$

Explanation for result



The local diffusion equilibrium is replaced by a non-local equilibrium.

Generalization to an Extended Object of small thickness (Clear Layer)

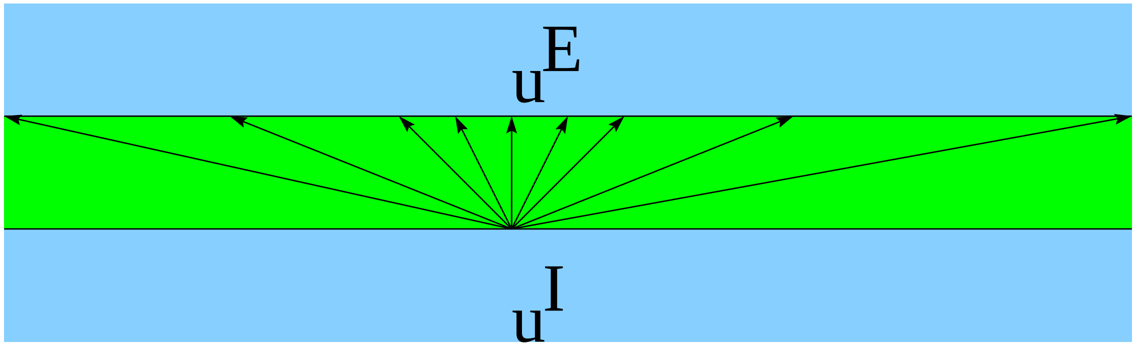


Geometry of the Clear Layer Ω^C of boundary $\begin{cases} \Sigma^E = \Sigma + lL_\varepsilon \nu(x), \\ \Sigma^I = \Sigma - lL_\varepsilon \nu(x), \end{cases}$
where $\nu(x)$ is the outgoing normal to Σ at $x \in \Sigma$.

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

Modified Equilibrium

We denote by $\mathcal{R}_\varepsilon^c$ the response operator that maps the incoming conditions on Γ_-^C to the outgoing distribution on Γ_+^C.



Postulate: The clear layer is thin enough so as not to modify the diffusion equilibrium at order $O(1)$, i.e.,

$$\mathcal{R}_\varepsilon^c = I_\varepsilon + \varepsilon \mathcal{R}_{1\varepsilon}^c.$$

Generalized Diffusion Equations with non-local interface conditions

Assume that $\mathcal{R}^c_{1\varepsilon}$ is $O(1)$ for smooth functions. The solution u_ε is then approximated, up to an error of order ε, by the solution of the following ε-dependent diffusion equation with non-local interface conditions:

$$\begin{aligned}
&-\text{div} D(x)\cdot\nabla u_0^\varepsilon(x) + \sigma_a(x) u_0^\varepsilon(x) = 0 \qquad \text{in } \Omega\backslash\Omega_\varepsilon^C\\
&u_0^\varepsilon(x) = \Lambda(g(x,v)) \qquad \text{on } \partial\Omega\\
&[[u_0^\varepsilon]] = 0 \qquad \text{on} \qquad \Sigma^E\\
&[\nu\cdot D\nabla u_0^\varepsilon] = K_\varepsilon(u_0^\varepsilon) \qquad \text{on} \qquad \Sigma^E,
\end{aligned}$$

$$[[u]](x^E) = u(x^E) - u(x^I) \qquad \text{and} \qquad [u](x^E) = u(x^E) - J(x^I)u(x^I),$$

$$\boxed{\begin{aligned}
K_\varepsilon u(x^E) \;&=\; \int_{v\cdot\nu_E(x^E)>0} v\cdot\nu_E(x^E)\,(\mathcal{R}^c_{1\varepsilon}u)(x^E,v)d\mu(v)\\
&+\; J(x^I)\int_{v\cdot\nu_I(x^I)>0} v\cdot\nu_I(x^I)\,(\mathcal{R}^c_{1\varepsilon}u)(x^I,v)d\mu(v) \qquad x^E\in\Sigma^E,
\end{aligned}}$$

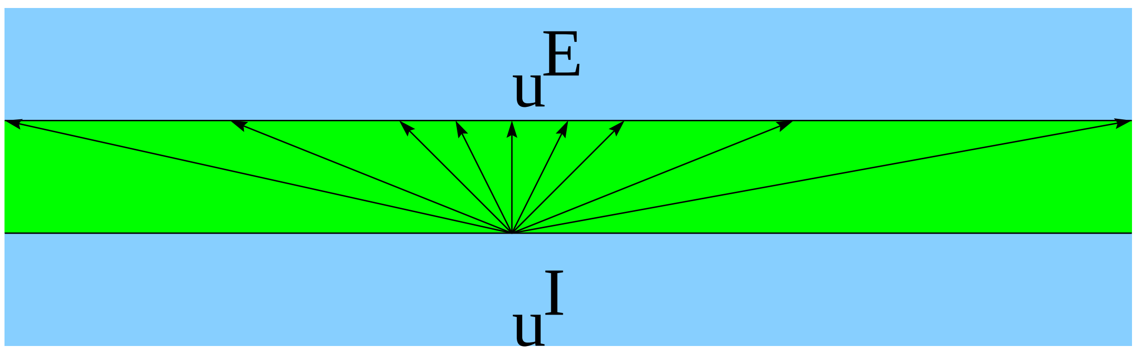
where the Jacobian of $x \mapsto x + 2lL_\varepsilon\nu(x)$ is $J(x) = |\det(I + 2lL_\varepsilon\nabla_x\nu(x))|$.

Application to Straight Clear Layers

It remains to verify *when* the corrector $\mathcal{R}^c_{1\varepsilon}$ is of order 1. In the case of a non-scattering clear layer with constant absorption, solving the free transport equation yields

$$\mathcal{R}^c_\varepsilon u(x,v) = e^{-\sigma^c_{a\varepsilon} t(x,v)} u(\bar{x},v).$$

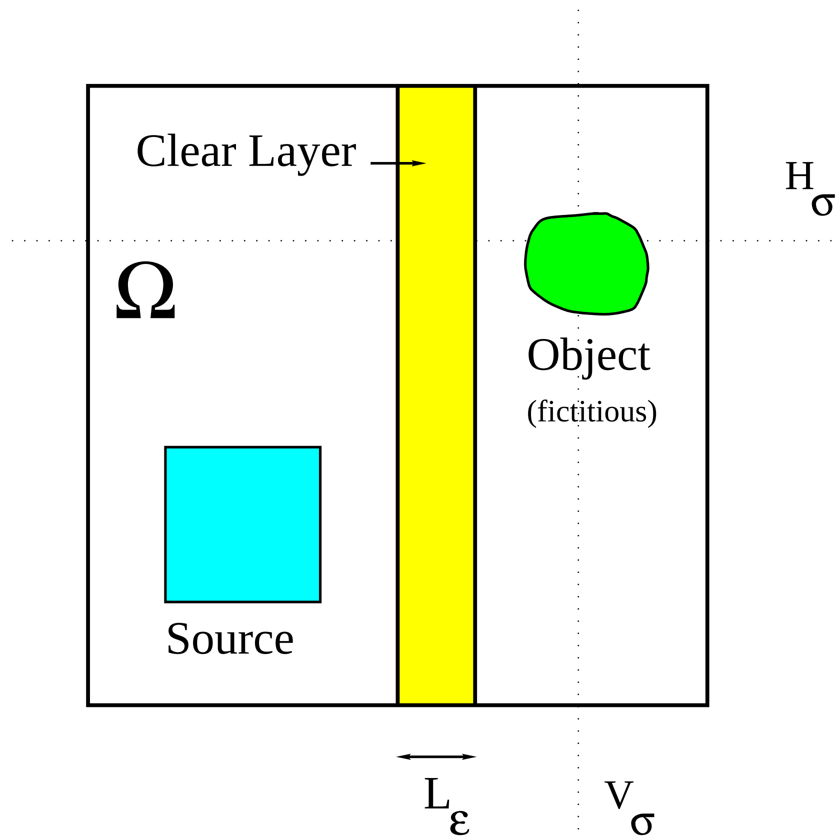
Here, $t(x,v)$ is the travel time, and $\bar{x} = \bar{x}(x,v) = x - t(x,v)v \in \partial\Omega^C_\varepsilon$.



After calculations, we obtain that $\mathcal{R}^c_{1\varepsilon}$ is of order 1 if L_ε and $\sigma^c_{a\varepsilon}$ verify

$$L_\varepsilon{}^2 |\ln L_\varepsilon| = \varepsilon \qquad \text{and} \qquad \sigma^c_{a\varepsilon} = \frac{\varepsilon}{L_\varepsilon} \sigma^c_a.$$

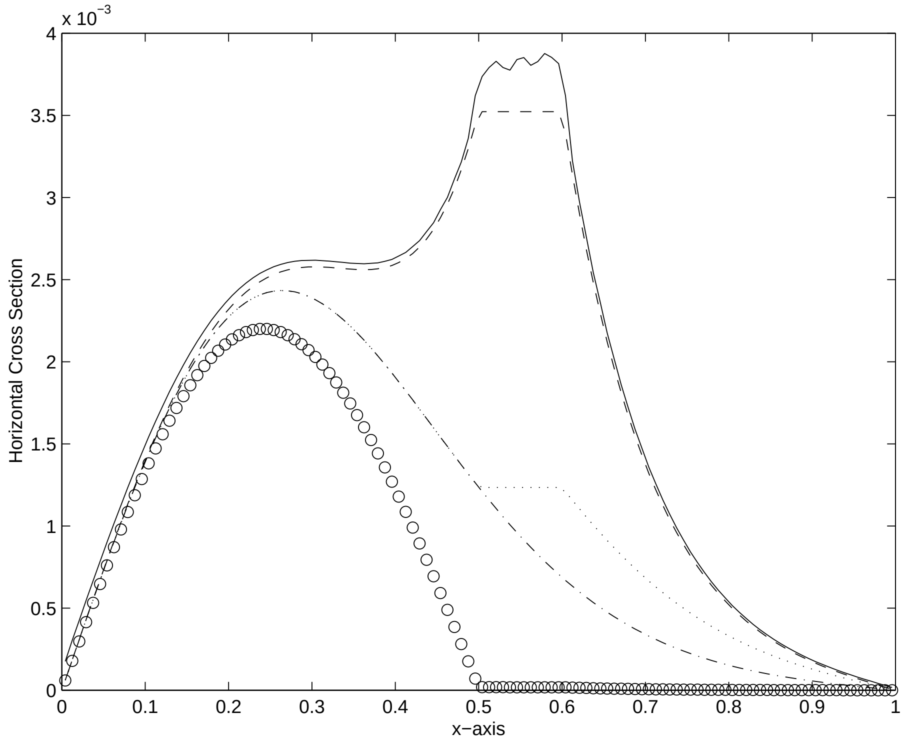
Numerical Application

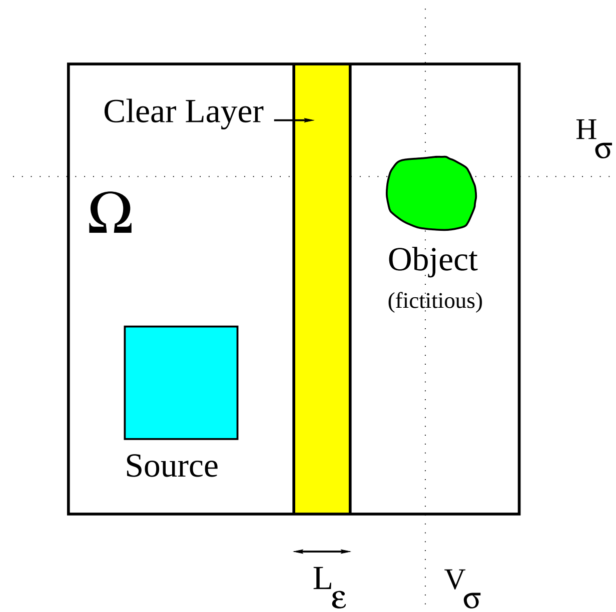


The domain is diffusive except within the clear layer.

The mean free path $\varepsilon = 0.01$ and the thickness $L_\varepsilon = 0.1$.

Horizontal cross-section of the solution





Horizontal cross section of the velocity average of the transport solution (solid line) and the generalized diffusion model (dashed line), the classical diffusion model (circles), and two models that neglect the clear layer.

Localization of interface conditions

The non-local interface conditions render the generalized diffusion model still computationally expensive.

We can localize the interface conditions as follows:

$$K_\varepsilon U(x) = -\nabla_\perp d^c \nabla_\perp U(x) + \sigma_a^c U(x) + \text{ smaller terms.}$$

Here, $\nabla_\perp$ is the tangential gradient operator along Σ.

Local Generalized Diffusion Model

The generalized diffusion model takes then the form (assuming the clear layer is non-absorbing)

$$-\nabla \cdot D(x)U(x) + \sigma_a(x)U(x) = 0 \qquad \text{in } \Omega\backslash\Sigma$$

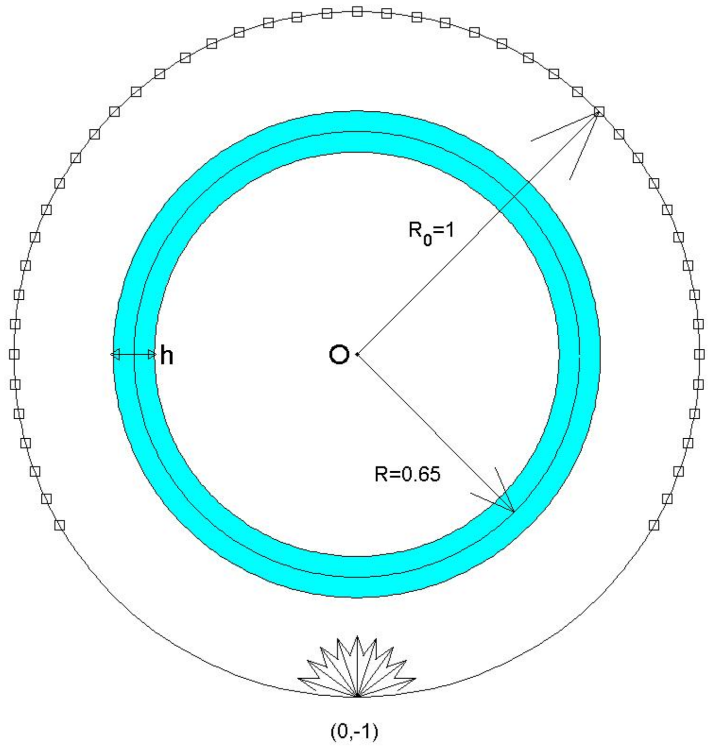
$$U(x) + 3L_3\varepsilon D(x)\nu(x)\cdot\nabla U(x) = \Lambda(g(x,v)) \qquad \text{on } \partial\Omega$$

$$[U](x) = 0 \qquad \text{on } \Sigma$$

$$[\nu \cdot D\nabla U](x) = -\nabla_\perp d^c \nabla_\perp U,$$

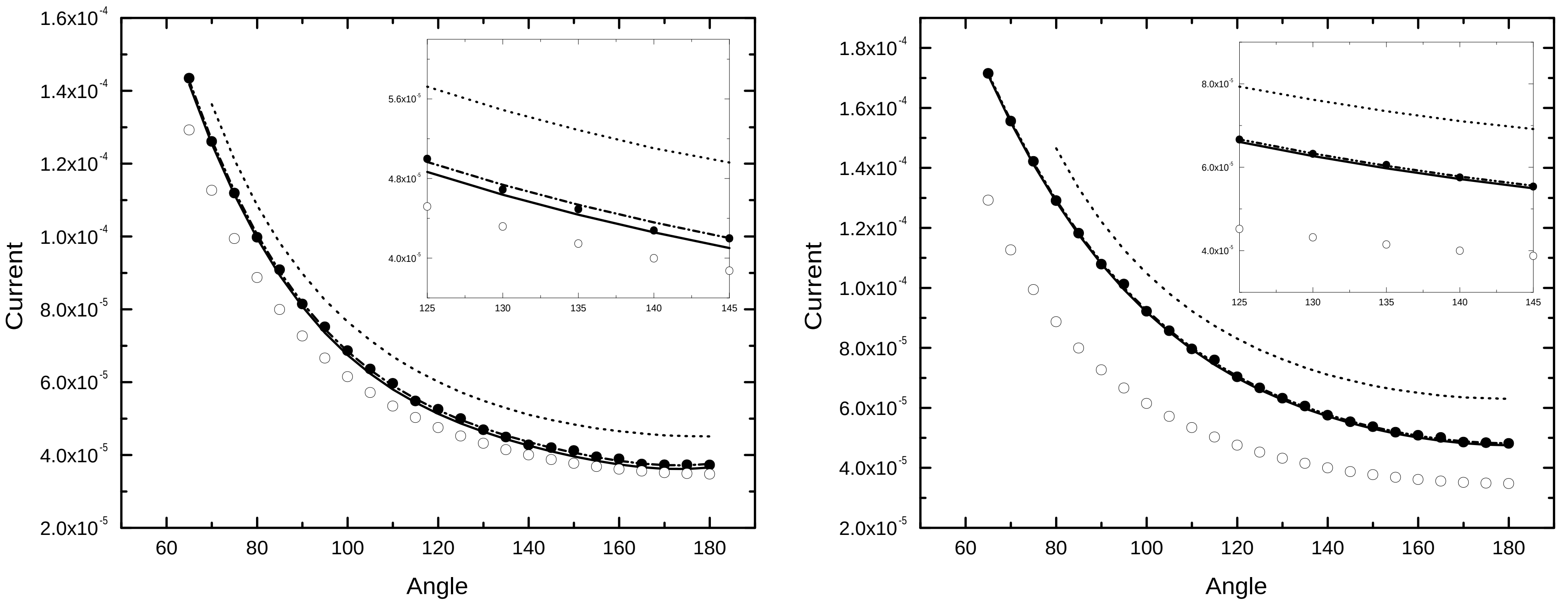
The approximation (w.r.t. transport solution) is of order $\sqrt{\varepsilon}$ when Σ has positive curvature and can be as bad as $|\ln\varepsilon|^{-1}$ for straight clear layers.

Numerical simulations



Geometry of domain with circular/spherical clear layer.

Two-dimensional Numerical simulation



Outgoing current for clear layers of 2 and 5 mean free paths.

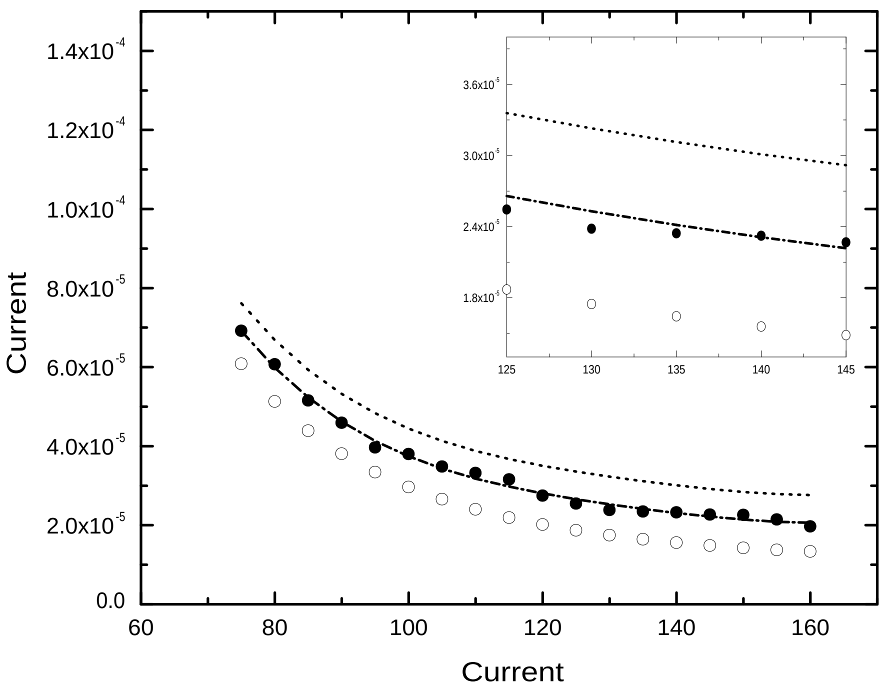
COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

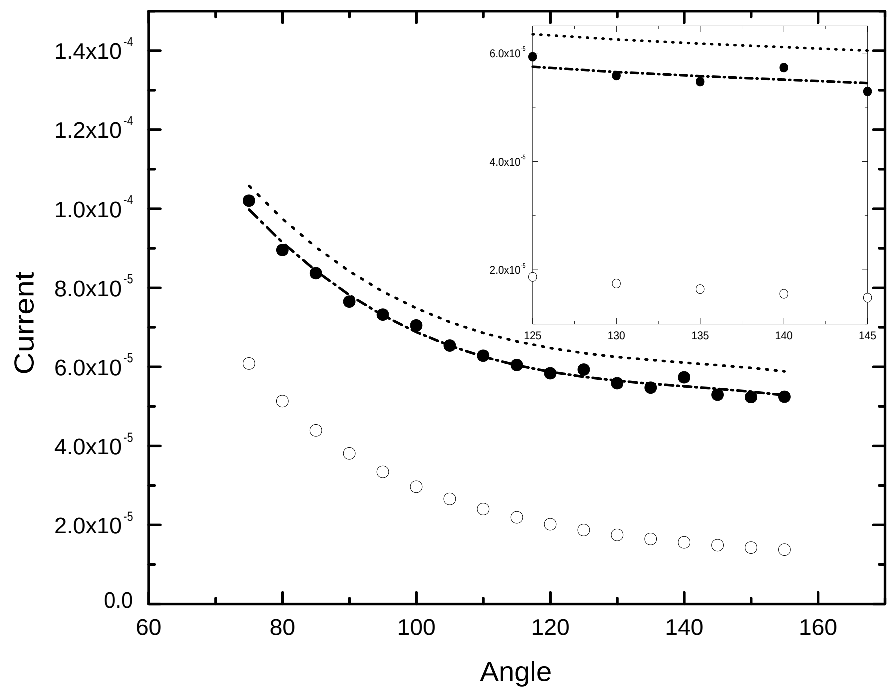
Two-dimensional Numerical simulation

h	0.01	0.02	0.03	0.04	0.05	0.06	0.07
d^C_{theory}	0.0124	0.0455	0.0971	0.166	0.253	0.355	0.475
$d^C_{\text{best fit}}$	0.0129	0.0465	0.0983	0.167	0.253	0.356	0.474
E_{GDM} (%)	1.17	1.56	1.43	1.09	0.81	0.56	0.60
E_{BF} (%)	0.73	0.65	0.57	0.49	0.46	0.47	0.46
E_{DI} (%)	3.3	10.2	17.7	24.5	30.2	35.3	39.8

Tangential diffusion coefficients and relative L^2 error between the transport Monte Carlo simulations and the various diffusion models for several thicknesses of the clear layer.

Three-dimensional Numerical simulation





Outgoing current for clear layers of 3 and 6 mean free paths.

Conclusions

- We have a macroscopic model that captures particle propagation *both* in scattering and non-scattering regions, such as embedded objects and clear layers.
- The generalized diffusion model is computationally only slightly more expensive than the classical diffusion equation (essentially, one term is added in the variational formulation) and much less expensive than the full phase-space transport model.
- The accuracy of the macroscopic equation is sufficient to address the inverse problem where absorption and scattering cross sections are reconstructed from boundary measurements.