# Laplacian Eigenfunctions in NMR

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IPAM Workshop « Laplacian Eigenvalues and Eigenfunctions »
February 9-13, 2009, Los Angeles CA, USA

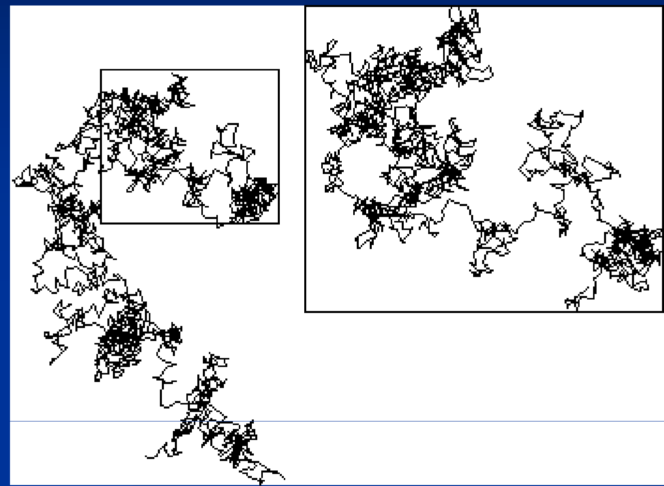
# Outline of the talk

- How to describe restricted diffusion?
- How to monitor restricted diffusion?
- Laplacian eigenfunctions in NMR
- Other applications
- Localization of eigenfunctions
- Conclusion and open questions

Grebenkov, Rev. Mod. Phys. 79, 1077 (2007); CMR 32A (2008)

# That amazing diffusion…

*Random walk of a "blind" particle*



Main transport mechanism:

- biology and physiology
- chemistry (heterogeneous catalysis)
- building industry (cement, concrete)

# Three kinds of problems

- FORWARD PROBLEM:

  What are the transport properties in a known geometry?

- INVERSE PROBLEM:

  What kind of geometrical information can be extracted from measurable transport properties?

  M. Kac : *Can one hear the shape of a drum?*

- OPTIMIZATION PROBLEM:

  What is the optimal geometry for a better realization of chosen transport properties?

# How to describe diffusion?

Probabilistic description

Microscopic or « individualistic » approach

# How to describe diffusion?

**Probabilistic description**

Microscopic or « individualistic » approach

**PDE description**

Macroscopic or « collective » approach

**Spectral description**

Global approach

$$c(\vec{r}, t)$$

$$\frac{\partial c}{\partial t} = D \Delta c$$

$$c(\vec{r}, 0) \doteq \rho(\vec{r})$$

$$D \frac{\partial c}{\partial n} + Kc = 0$$

# How to describe diffusion?

**Probabilistic description**

Microscopic or « individualistic » approach

Monte Carlo

**PDE description**

Macroscopic or « collective » approach

Finite differences

**Spectral description**

Global approach

Finite elements

$$\{u_m(\vec{r})\}$$

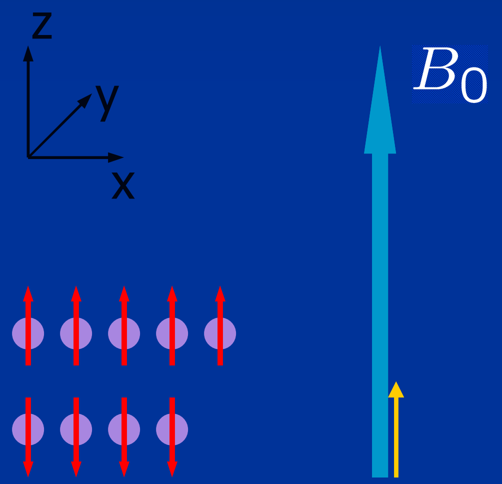
$$-\Delta u_m = \lambda_m u_m$$

$$D\frac{\partial u_m}{\partial n} + K u_m = 0$$

# How to monitor restricted diffusion?

# Schematic principle of NMR

Static magnetic field $B_0$

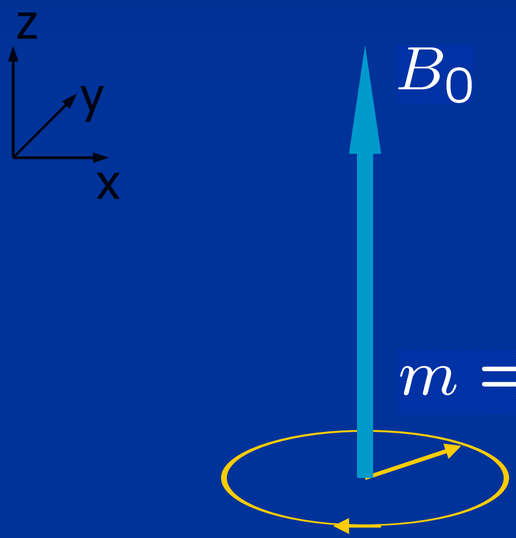



local magnetization

90° rf pulse

# Schematic principle of NMR

Static magnetic field $B_0$




$B_0$

$$m = m_x + i m_y \propto e^{i\varphi}$$

$$\omega = \gamma B_0$$

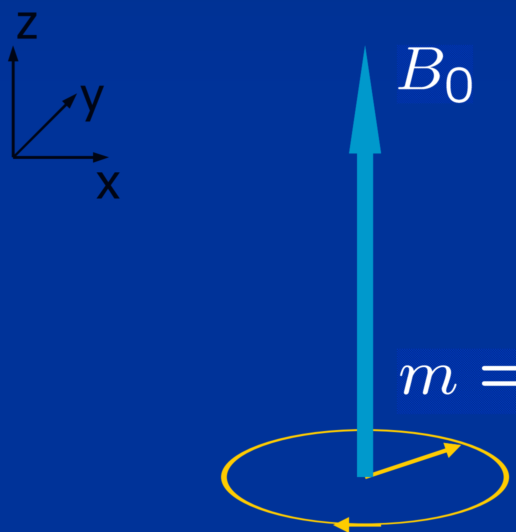
Phase at time T

$$\varphi_0 = \gamma B_0 T$$

# Schematic principle of NMR

Static magnetic field $B_0$

Time-dependent linear magnetic field gradient




$m = m_x + i m_y$

$\propto e^{i\varphi}$

Total transverse magnetization:

$$S \propto \mathbb{E}\{e^{i\varphi}\}$$

$$\omega = \gamma B_0$$

$$\omega(\vec{r}, t) = \gamma B(\vec{r}, t)$$

Phase at time T

$$\varphi_0 = \gamma B_0 T$$

$$\varphi = \int_0^T dt \; \gamma B(\vec{r}(t), t)$$

# Schematic principle of NMR

Bloch-Torrey equation

time evolution — diffusion — gradient encoding

$$\left(\frac{\partial}{\partial t} - D\Delta + i\gamma B(\vec{r}, t)\right) \mathfrak{m}(\vec{r}, t) = 0$$

magnetization

$\mathfrak{m}(\vec{r}, 0) = \rho(\vec{r})$ initial condition (e.g., uniform)

$D\frac{\partial}{\partial n}\mathfrak{m}(\vec{r}, t) + W\mathfrak{m}(\vec{r}, t) = 0$ boundary condition

$S = \int d\vec{r}\ \mathfrak{m}(\vec{r}, T)$ macroscopic signal

Torrey, Phys. Rev. 104, 563 (1956)

# Matrix formalism with Laplacian eigenfunctions

Robertson, Phys. Rev. 151, 273 (1966)
Caprihan, Wang, Fukushima, J. Magn. Reson. A118, 94 (1996)
Callaghan, J. Magn. Reson. 129, 74 (1997)
Barzykin, Phys. Rev. B 58, 14171 (1998); JMR 139, 342 (1999)
Axelrod, Sen, J. Chem. Phys. 114, 6878 (2001)
Grebenkov, Rev. Mod. Phys. 79, 1077 (2007); Conc. Magn. Reson. 32A (2008)

# Time-independent magnetic field

$$\left(\frac{\partial}{\partial t} - D\Delta + i\gamma B(\vec{r})\right)\mathfrak{m}(\vec{r},t) = 0$$

$$D\frac{\partial \mathfrak{m}}{\partial n} + \ldots$$

$$\mathfrak{m}(\vec{r},0) \ldots \rho(\vec{r})$$

D, γ and K are the parameters

$$\Lambda_{m,m'} = \delta_{m,m'}\ \lambda_m$$

$$\mathcal{B}_{m,m'} = \int_\Omega d\vec{r}\ u_m^*(\vec{r})\ B(\vec{r})\ u_{m'}(\vec{r})$$

$$\ldots(t)\, u_m(\vec{r})$$

$$\left(\frac{\partial}{\partial t} + D\Lambda + i\gamma\mathcal{B}\right)C(t) = 0$$

$$C(t) = \begin{pmatrix} c_0(t) \\ c_1(t) \\ c_2(t) \\ c_3(t) \\ \ldots \end{pmatrix}$$

$$C(t) = C(0)\exp[-(D\Lambda + i\gamma\mathcal{B})t]$$

# Time-independent magnetic field

$$S = \int_\Omega d\vec{r}\ \mathfrak{m}(\vec{r},t) = \sum_m c_m(t) \underbrace{\int_\Omega d\vec{r}\ u_m(\vec{r})}_{\tilde{U}_m}$$

$$\mathfrak{m}(\vec{r},0) = \sum_m c_m(0) u_m(\vec{r})$$

$\rho(\vec{r})$

$$c_m(0) = \int d\vec{r}\ \rho(\vec{r})\ u_m^*(\vec{r})$$

$$S = (U \ \ \exp[-(D\Lambda + i\gamma\mathcal{B})t]\ \tilde{U})$$

$$C(t) = C(0) \exp[-(D\Lambda + i\gamma\mathcal{B})t]$$

# Matrix product "rule":

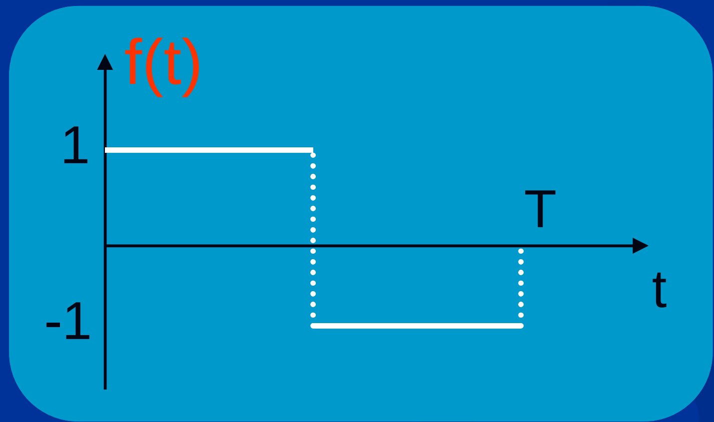
$$S = (U \ \exp[-(D\Lambda + i\gamma\mathcal{B})t] \ \tilde{U})$$

Initial magnetization

Evolution operator for diffusion and encoding

Averaging over all the nuclei

Free Induction Decay (FID)




Spin-echo signal

CPMG echo train

$$S_n = (U\left[e^{-(D\Lambda+i\gamma\mathcal{B})t/2} \ e^{-(D\Lambda-i\gamma\mathcal{B})t/2}\right]^n \tilde{U})$$

# Matrix product "rule":

$$S = \left(U \ \exp[-(D\Lambda + i\gamma \mathcal{B})t] \ \tilde{U}\right)$$

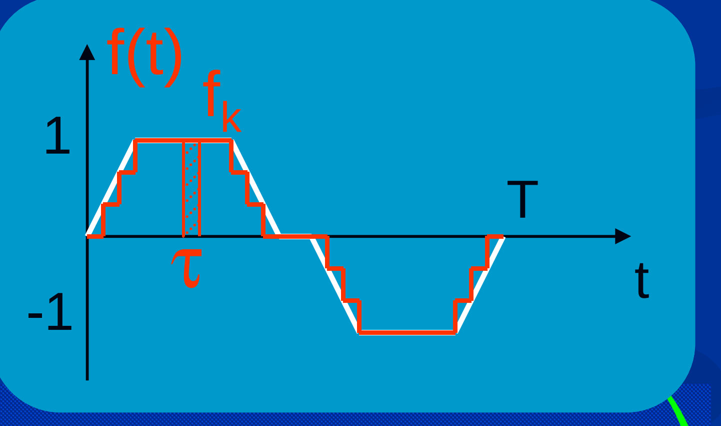
Initial magnetization

Evolution operator for diffusion and encoding

Averaging over all the nuclei

Free Induction Decay (FID)

Arbitrary temporal profile?




$$S \approx \left(U \ \prod_{k=0}^{N} e^{-(D\Lambda + i\gamma f_k \mathcal{B})\tau} \ \tilde{U}\right)$$

# Matrix B: weighted correlations

$$\Lambda_{m,m'} = \delta_{m,m'} \ \lambda_m$$

$$\mathcal{B}_{m,m'} = \int_{\Omega} d\vec{r} \ u_m^*(\vec{r}) \ B(\vec{r}) \ u_{m'}(\vec{r})$$

Unit interval

$$u_m(x) = cos(\pi m x)$$

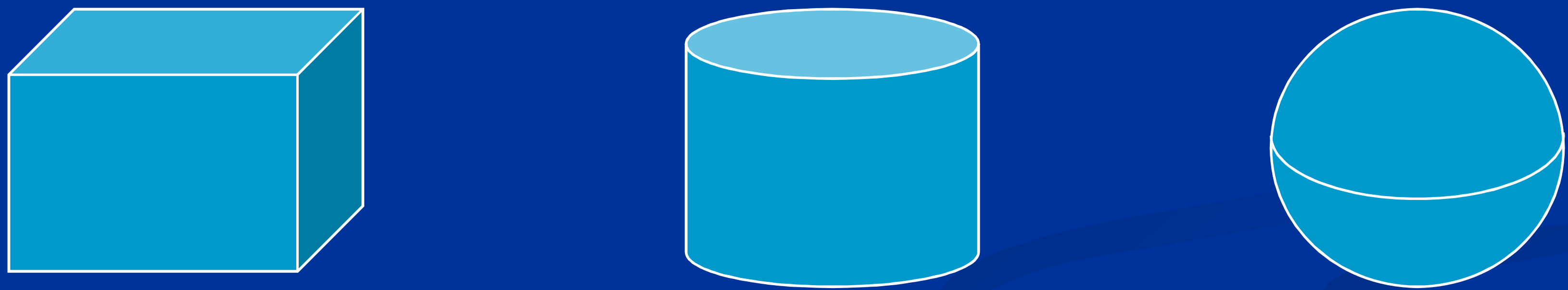
$$B_{m,m'} = \frac{1}{2}(a_{m+m'} + a_{m-m'})$$

$$a_m = \int_0^1 dx \ B(x) \ \cos(\pi m x)$$

# Computation for simple shapes

$$\Lambda_{m,m'} = \delta_{m,m'}\ \lambda_m$$

$$\mathcal{B}_{m,m'} = \int_{\Omega} d\vec{r}\ u_m^*(\vec{r})\ B(\vec{r})\ u_{m'}(\vec{r})$$



$\cos(z)$ $\qquad$ $J_n(z)$ $\qquad$ $j_n(z)$

$$\mathcal{B}_{m,m'} = [(-1)^{m+m'} - 1]\frac{\epsilon_m \epsilon_{m'}}{\pi^2}\ \frac{m^2 + m'^2}{(m^2 - m'^2)^2}$$

$$\Lambda_{m,m'} = \delta_{m,m'}\pi^2 m^2$$

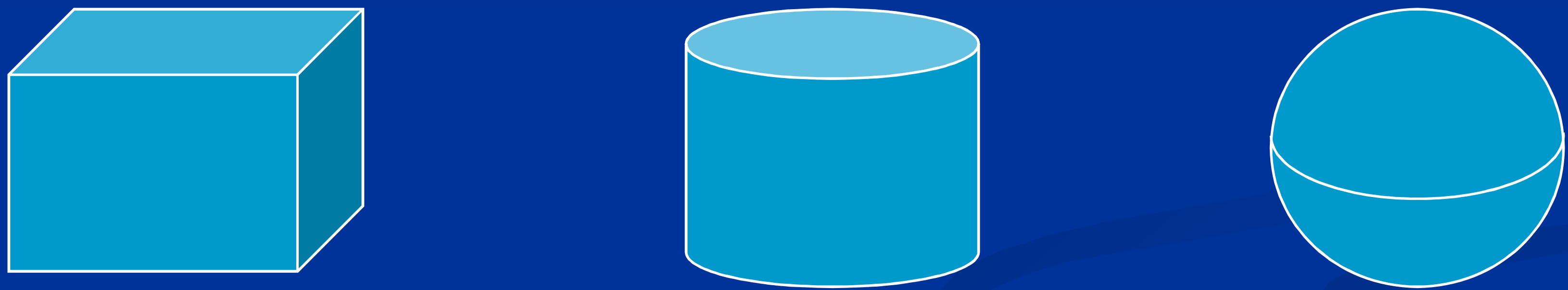
$$\epsilon_m = \sqrt{2 - \delta_{m,0}}$$

Barzykin, J. Magn. Reson. 139, 342 (1999)

# Computation for simple shapes

$$\Lambda_{m,m'} = \delta_{m,m'} \ \lambda_m$$

$$\mathcal{B}_{m,m'} = \int_{\Omega} d\vec{r} \ u^*_m(\vec{r}) \ B(\vec{r}) \ u_{m'}(\vec{r})$$



$\cos(z)$ $J_n(z)$ $j_n(z)$

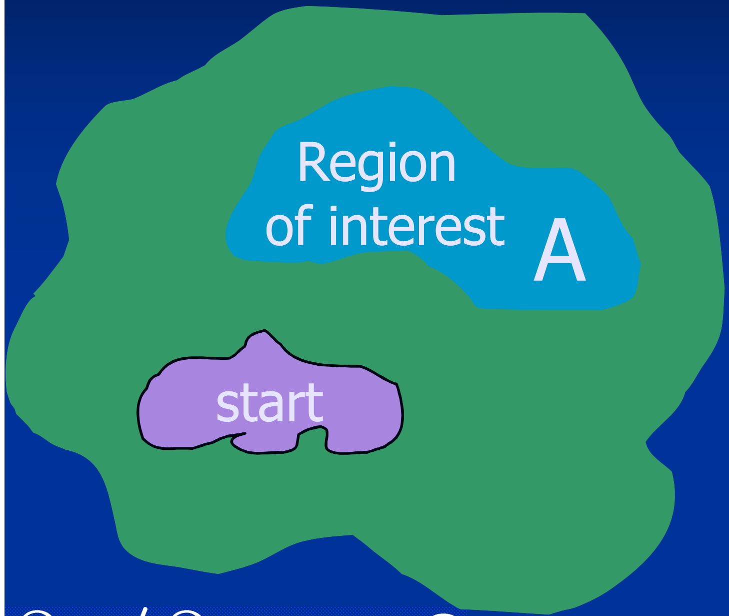
$$\mathcal{B}_{nk,n'k'} = \delta_{n,n'\pm 1} \sqrt{1 + \delta_{n,0} + \delta_{n',0}} \sqrt{\frac{\lambda_{nk}}{\lambda_{nk} - n^2}} \times \sqrt{\frac{\lambda_{n'k'}}{\lambda_{n'k'} - n'^2}} \ \frac{\lambda_{nk} + \lambda_{n'k'} - 2nn'}{(\lambda_{nk} - \lambda_{n'k'})^2}$$

Grebenkov,
Rev. Mod. Phys 79 (2007)

# Many other applications…

- Relaxation/trapping/reaction processes
- Residence and local times
- First passage/exit times
- Exchange processes

# Residence time distribution




$\varphi$

$$\Lambda_{m,m'} = \delta_{m,m'} \; \lambda_m$$

$$\mathcal{B}_{m,m'} = \int\limits_A d\vec{r} \; u^*_m(\vec{r}) \; u_{m'}(\vec{r})$$

Feynman-Kac formula

$$\mathbb{E}\{e^{-q\varphi}\} = \int\limits_\Omega d\vec{r} \; c(\vec{r},t)$$

$\partial c/\partial n = 0$

probability to find

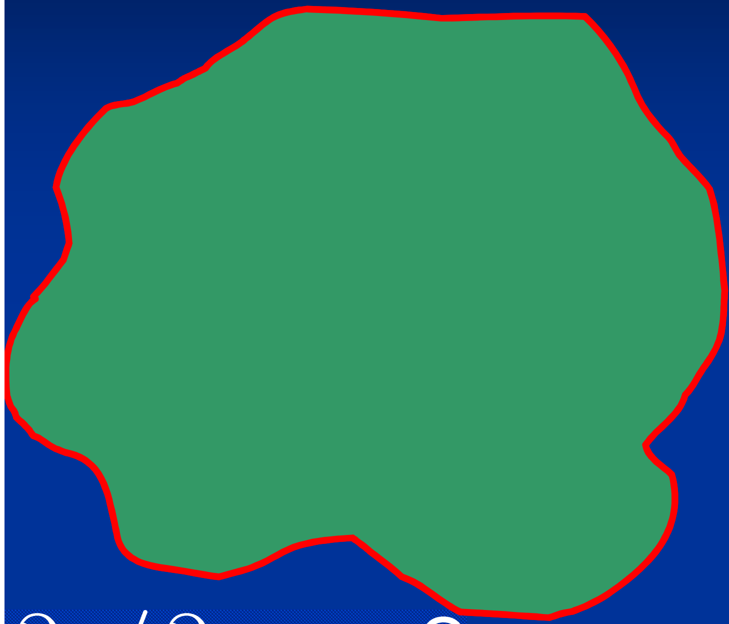
$c($

$$\mathbb{E}\{e^{-q\varphi}\} = (U \exp[-(D\Lambda + q\mathcal{B})t] \; \tilde{U})$$

$$\left(\frac{\partial}{\partial t} - D\Delta + q\mathbb{I}_A(\vec{r})\right) c(\vec{r},t) = 0$$

Grebenkov, PRE 76, 041139 (2007)

# Local time distribution



$\varphi$

$$\Lambda_{m,m'} = \delta_{m,m'}\ \lambda_m$$

$$\mathcal{B}_{m,m'} = \int\limits_{\partial\Omega} d\vec{r}\ u_m^*(\vec{r})\ u_{m'}(\vec{r})$$

Feynman-Kac formula

$$\mathbb{E}\{e^{-q\varphi}\} = \int\limits_{\Omega} d\vec{r}\ c(\vec{r},t)$$

survival probability

$\partial c/\partial n = 0$

$c($

$$\mathbb{E}\{e^{-q\varphi}\} = (U \exp[-(D\Lambda + q\mathcal{B})t]\ \tilde{U})$$

$$\left(\frac{\partial}{\partial t} - D\Delta + q\ \mathbb{I}_{\partial\Omega_\varepsilon}(\vec{r})/\varepsilon\right) c(\vec{r},t) = 0$$

Grebenkov, PRE 76, 041139 (2007)

# Superposition of attenuation mechanisms

- Surface and bulk relaxation

$$S = (U \exp[-(D\Lambda + i\gamma\mathcal{B} + W\tilde{B})t]\ \tilde{U})$$

- Magnetic field gradient encoding
- Dipole magnetic field (susceptibility)

These are independent attenuation mechanisms

⇩

Simple superposition in Bloch-Torrey equation

# Simple versus Complex?

Do we understand diffusion in complex geometries?

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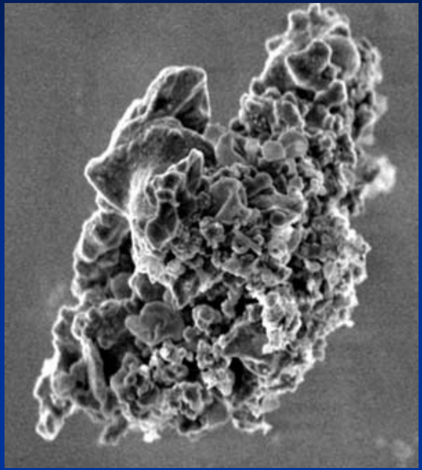
Many analytical and numerical results

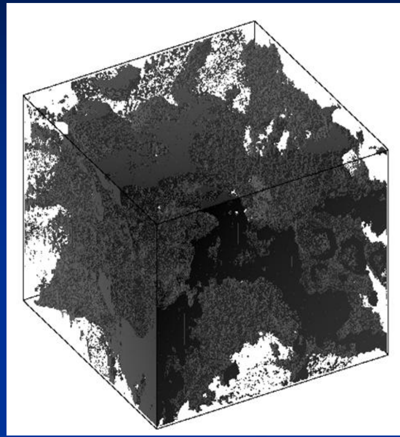
Grebenkov, Rev. Mod. Phys 79, 1077 (2007)

# Porous media…

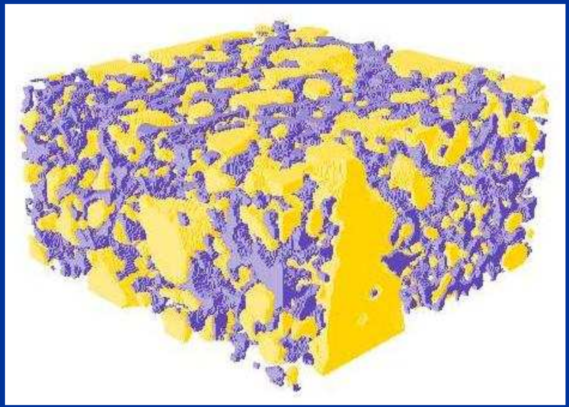
in material sciences



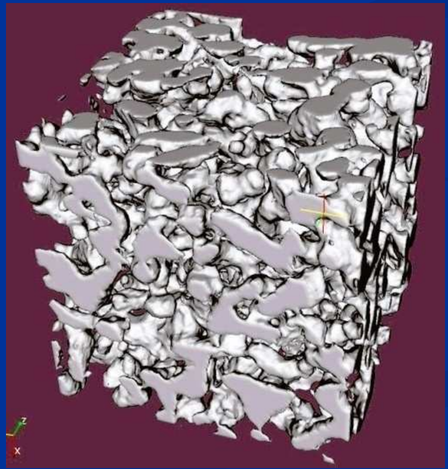
Stardust



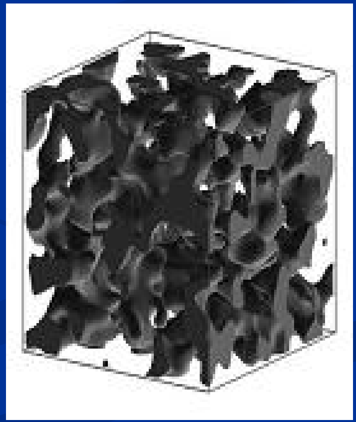
3D reconstruction
of a limestone



3D reconstruction
of a cement paste



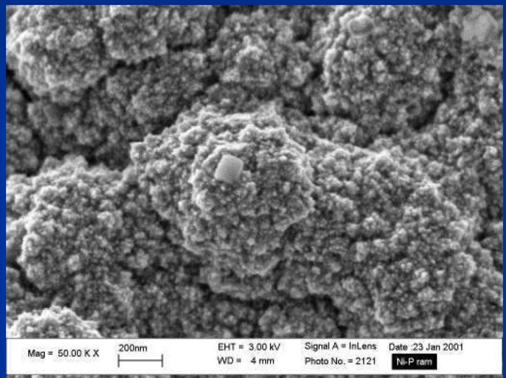
Micro-CT image
of a snow pack



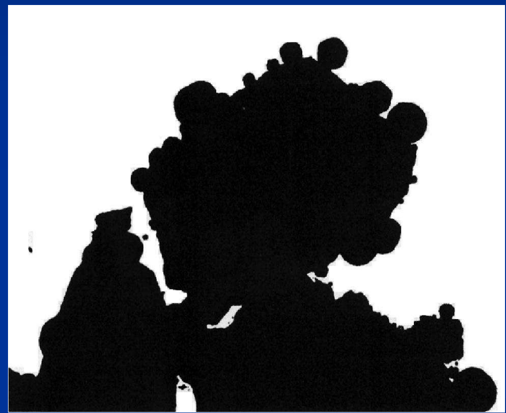
3D model of
Vycor glass

# Porous media…

## in chemistry and electrochemistry

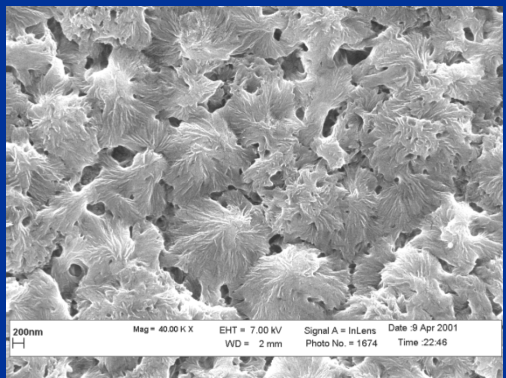



Microroughness of a nickel surface

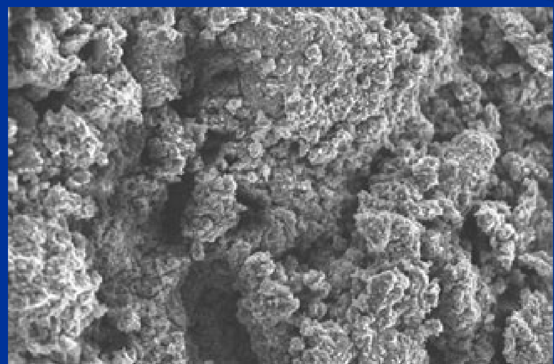


Typical shape of a porous catalyst

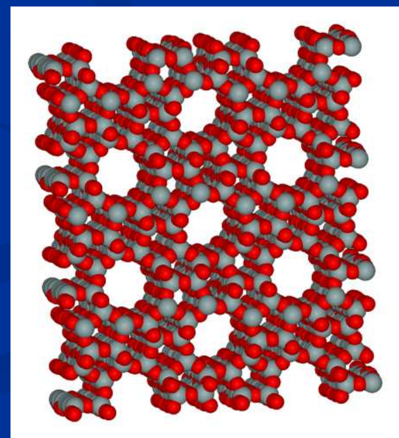
Copper dendrites




Nylon surface



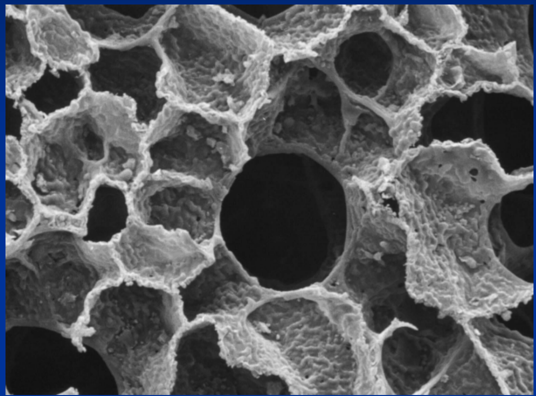
Porous polymer



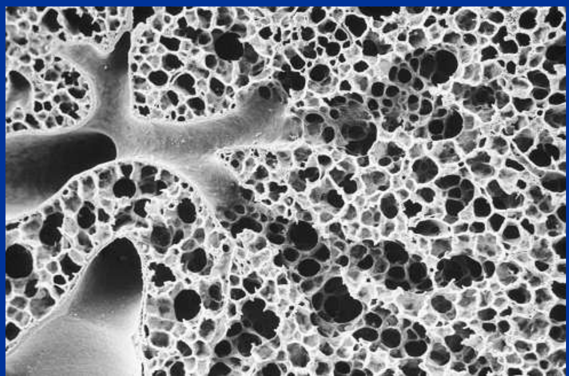
Zeolites

# Porous media…

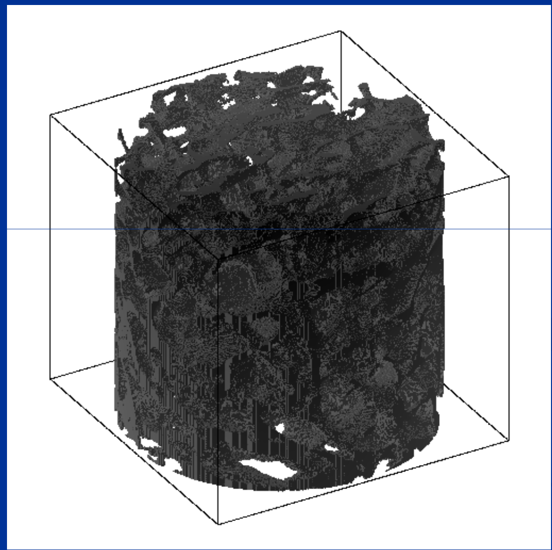
in physiology



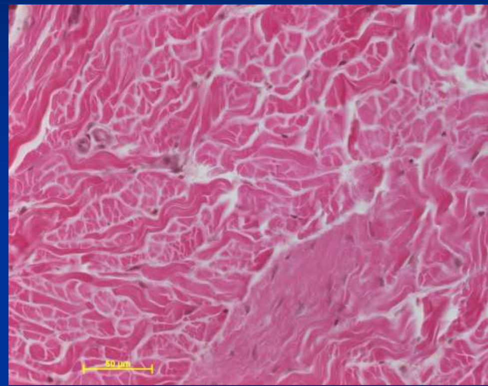
Lung acinus



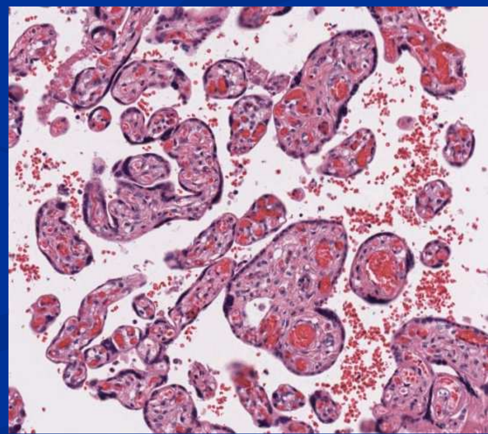
2D cut of a human acinus



3D tomography of a bone

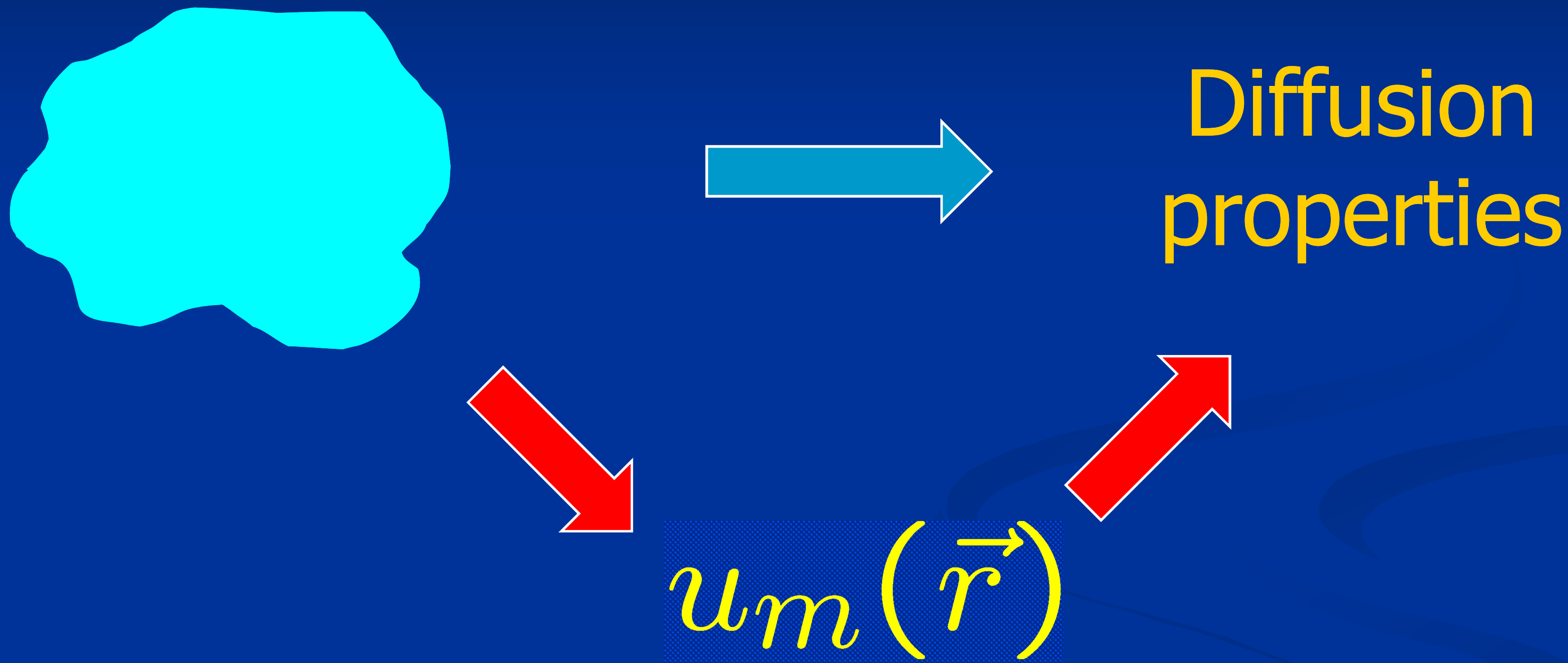


2D cut of a skin



2D cut of a human placenta

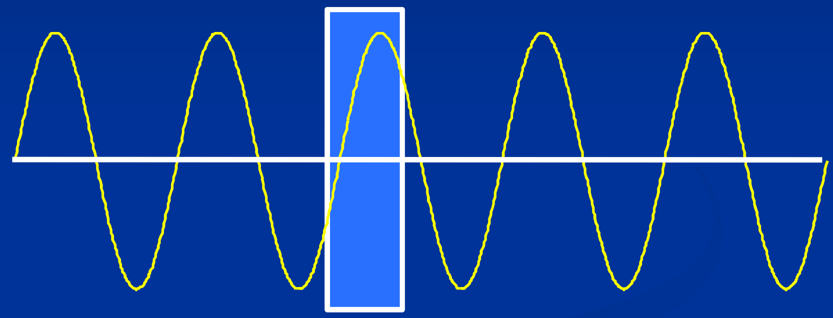
# Spectral insight



# Localization of eigenfunctions

"Regular" domains
(interval, disk, sphere)

$$u_m(x) = sin(\pi m x)$$

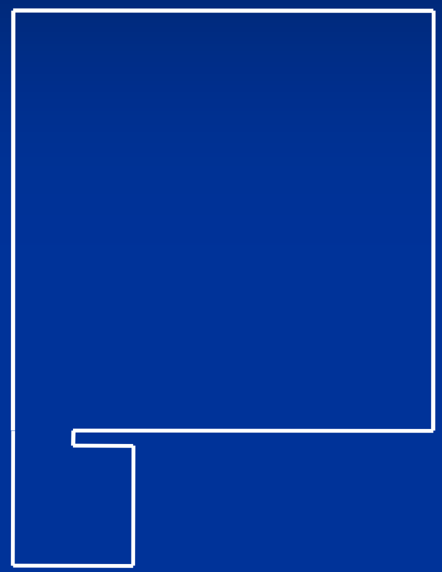


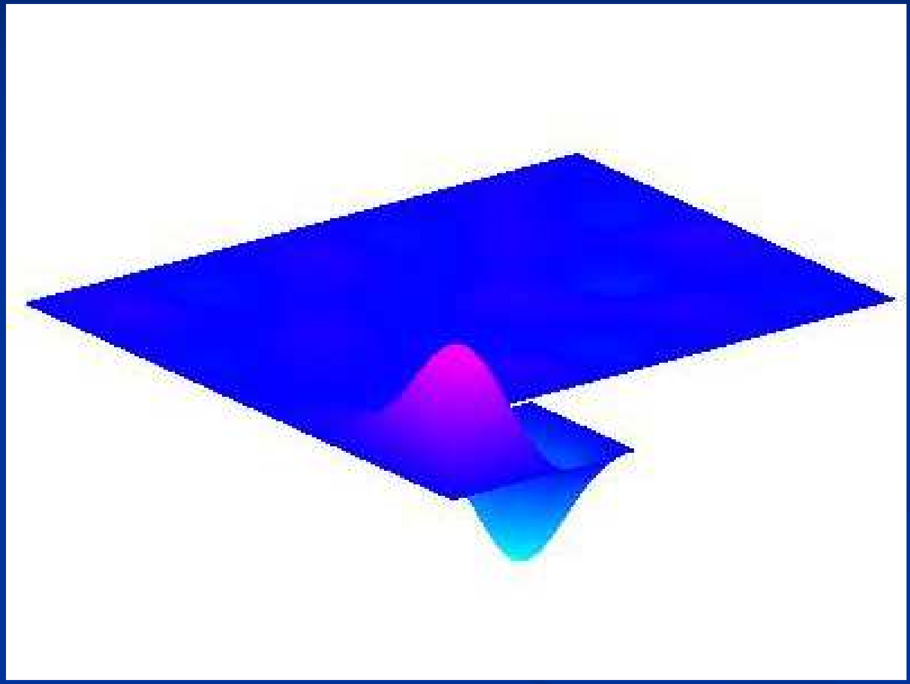
Nonlocalized (extended) eigenfunction:
Any compact subset of the domain supports a fraction of eigenfunction

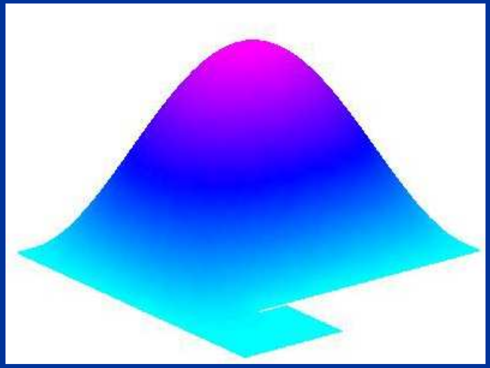
Localized eigenfunction:
There exists a small compact subset that supports a large fraction of eigenfunction

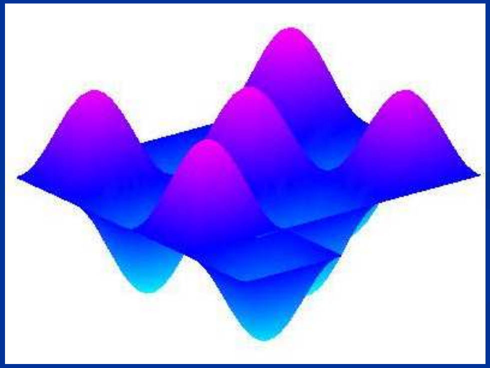
?

# Localization of eigenfunctions

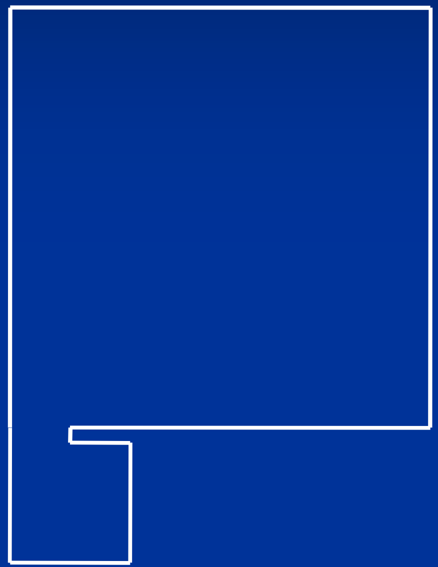








# Localization of eigenfunctions



Geometrical irregularity

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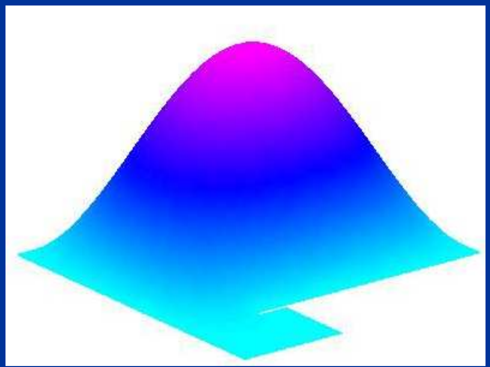
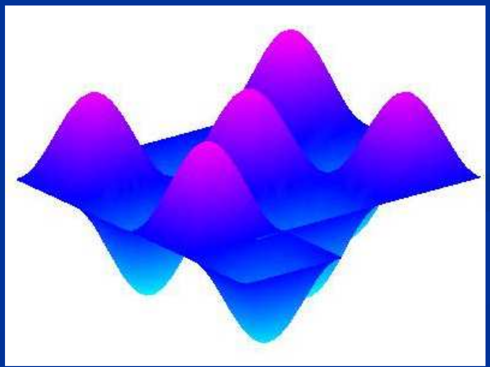
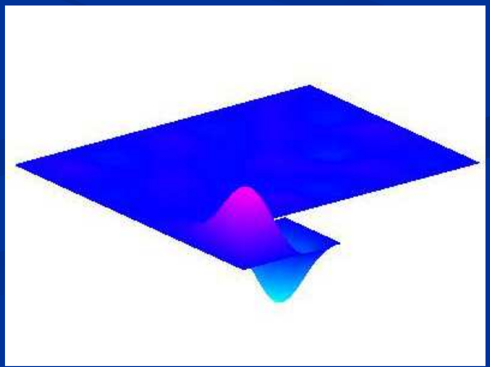
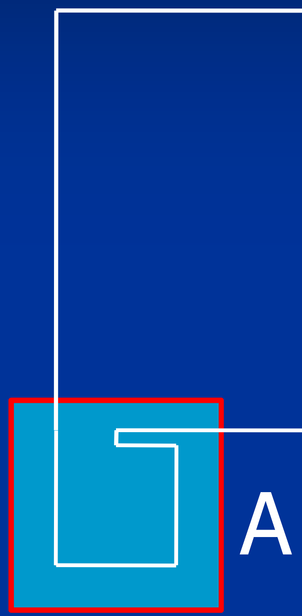
Localized eigenfunctions







# Localization of eigenfunctions

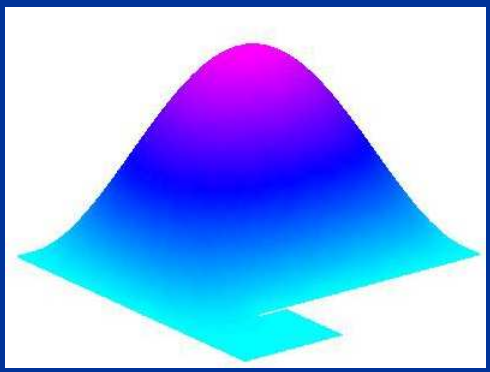


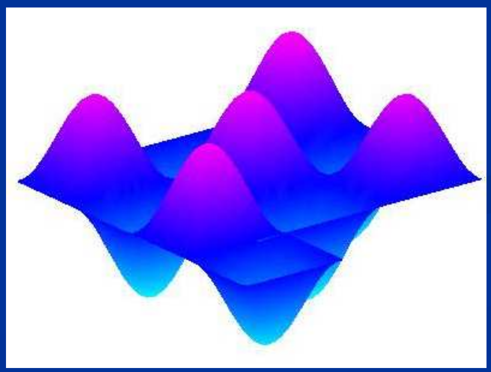

Trapping/exchange process

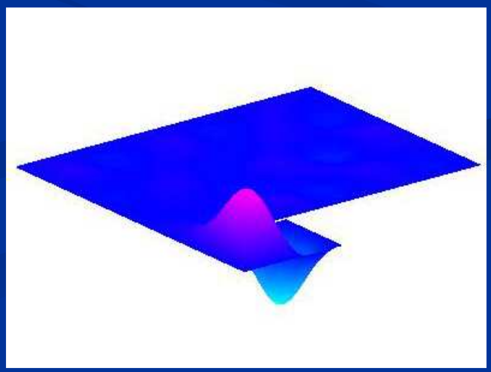
$$\Lambda_{m,m'} = \delta_{m,m'} \; \lambda_m$$

$$\mathcal{B}_{m,m'} = \int_A d\vec{r} \; u^*_m(\vec{r}) \; u_{m'}(\vec{r})$$

Particular structure of B







# Spectral approach: pro & contro

## Pro

- A complete description of restricted diffusion
- Easy implementation of various attenuation mechanisms
- Very accurate and rapid computation
- Possibility for profound theoretical analysis, investigation of different diffusion regimes, etc.

## Contro

- Computation of the Laplacian eigenfunctions in complex geometries is a difficult numerical task

http://pmc.polytechnique.fr/pagesperso/dg/MCF/MCF_e.htm

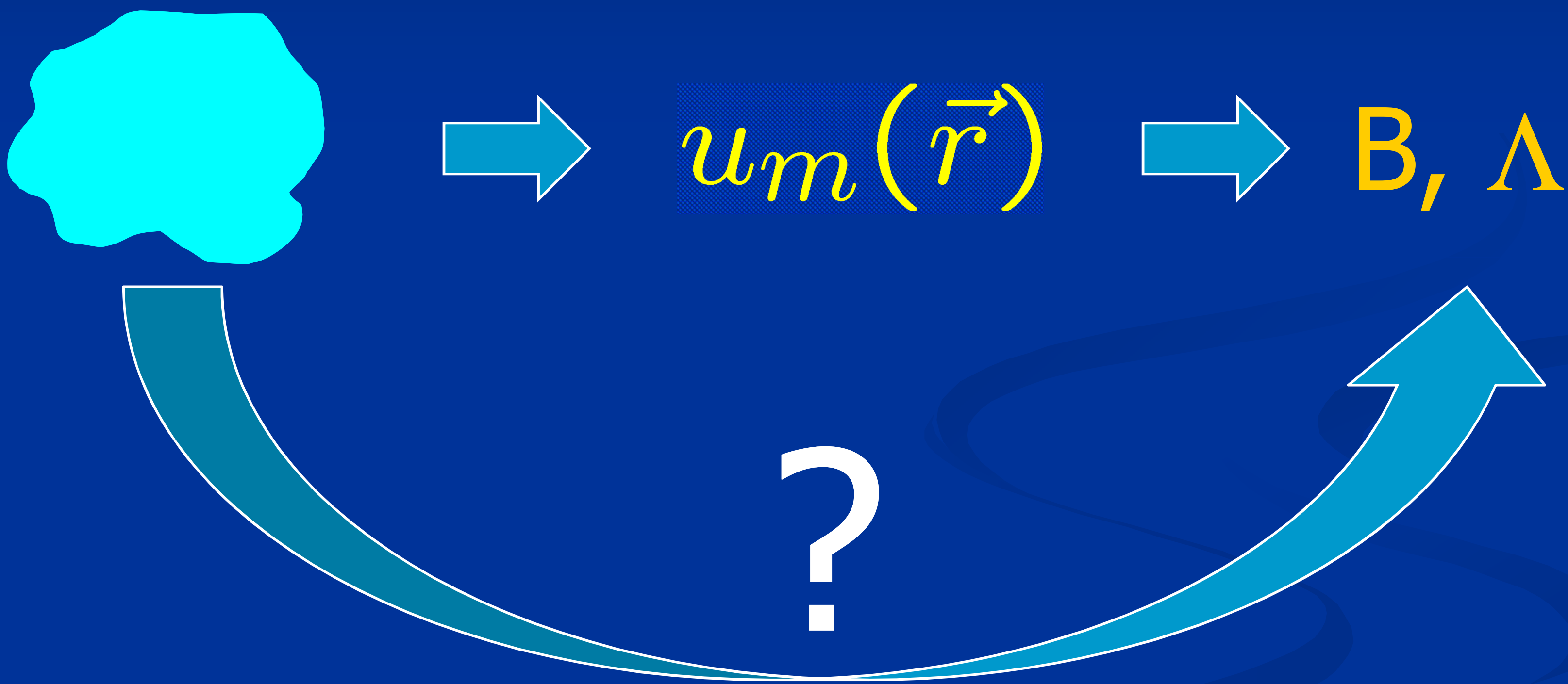
# Open questions

## Forward problem

- How does a complex geometry modify the signal and other related quantities?
- How does a complex geometry modify the Laplace operator eigenfunctions (e.g., the structure of the matrix B)?
- What is the role of localization in diffusion processes?

# Open questions

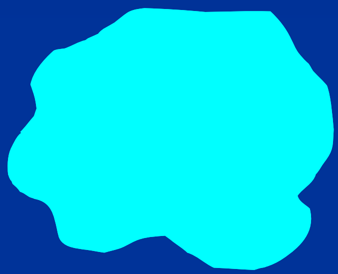
## Computational problem



# Open questions

## Inverse problem

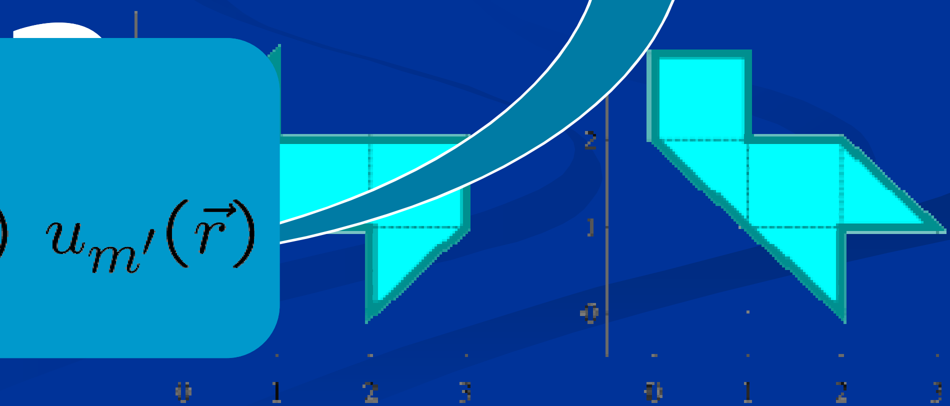
- Can one "hear" the shape of the lungs?



↔ B, Λ ↔ signal

$$\Lambda_{m,m'} = \delta_{m,m'}\ \lambda_m$$

$$\mathcal{B}_{m,m'} = \int_{\Omega} d\vec{r}\ u^*_m(\vec{r})\ B(\vec{r})\ u_{m'}(\vec{r})$$



Gordon et al., Bull. Am. Math. Soc. 27, 134 (1992)

# Main message

**We need efficient numerical techniques to calculate Laplacian eigenfunctions in complex model geometries, especially in 3D**

**Thank you for your attention!!!**

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