Diffusion et ondes dans les milieux à gradient de propriétés 1D. Construction de profils analytiquement solubles avec leurs solutions associées. Applications en CND thermique, optique des couches minces, et micro-météorologie

Journée SFT, 20 juin 2019

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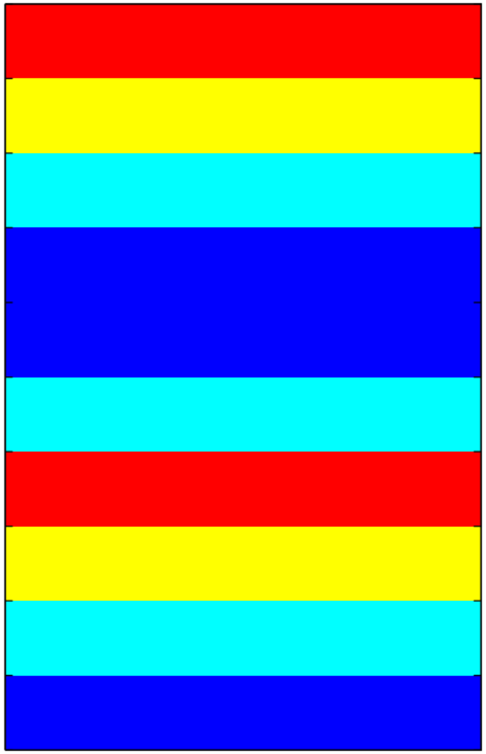
ONERA

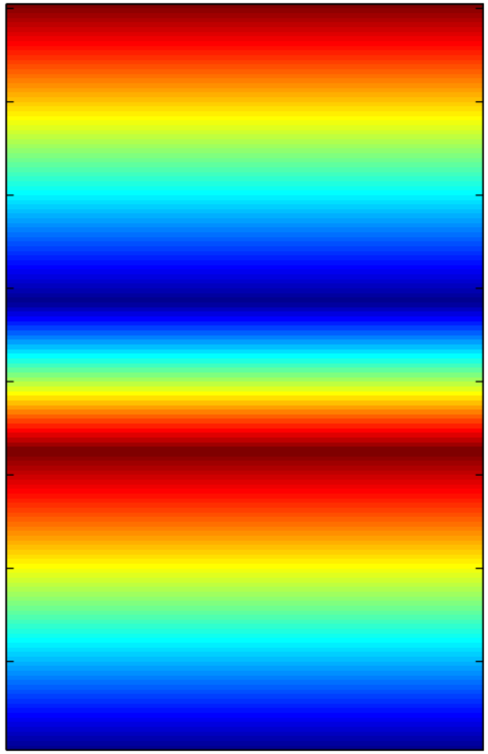
THE FRENCH AEROSPACE LAB

Foreword (1/5): Modeling of transfer phenomena in heterogeneous media

An analytical journey from

the world of **piece-wise constant** properties to the world of **continuous** properties



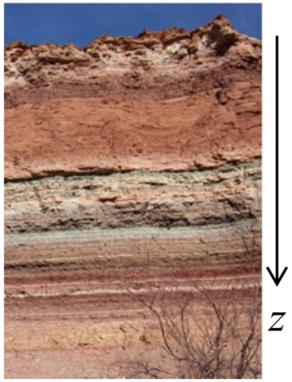


Foreword (2/5): Heat equation in graded media

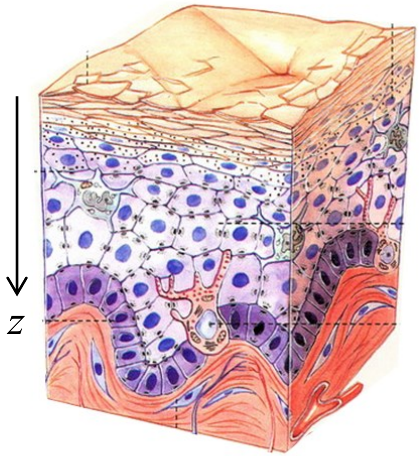
Heat equation for 1D **heat diffusion** in a **graded medium**

$$c(z)\frac{\partial T}{\partial t}=\frac{\partial}{\partial z}\left(\lambda(z)\frac{\partial T}{\partial z}\right)$$

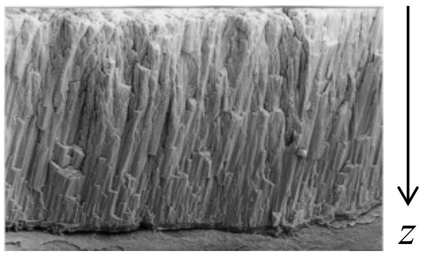
variable **volumetric heat capacity**   ***variable*** **thermal conductivity**



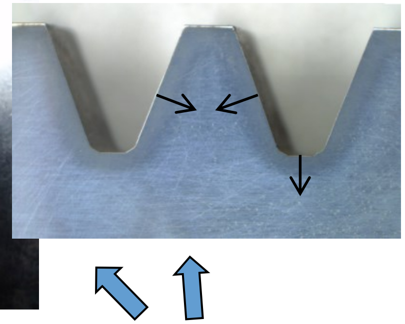
Soils



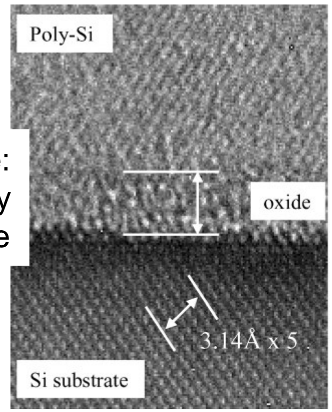
Skin



Thermal Barrier Coating



Gear teeth. Carburized **case-hardened** steel



Graded interface at nanoscale: Oxygen concentration in thermally grown ultrathin SiO_x gate oxide

Foreword (3/5): Other (diffusion) equations of the same form

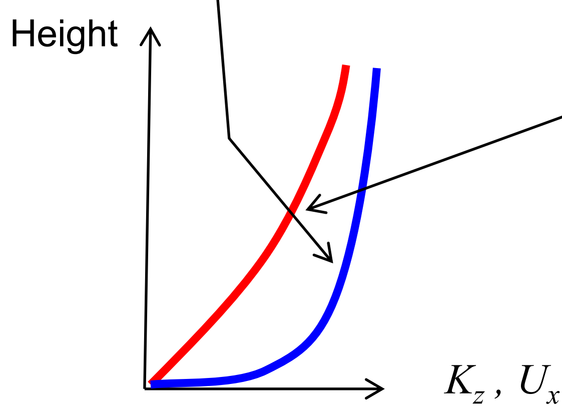
- Stationary, 2D, **advection-diffusion** equation :

$$U_x(z)\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C}{\partial z}\right)$$

e.g.: **pollutant dispersion** in the atmosphere

variable **wind speed**

variable **eddy diffusivity**



- **Matter diffusion** (Fick's law) with ***variable*** **diffusion coefficient**
- **Electric transmission lines (tapered *RC*** lines : ***R(z), C(z)*****)**
- **Graetz problem, etc…**

Foreword (4/5): Wave equations of "similar" form

EM waves (Maxwell's equations)

$$-\omega^2 \varepsilon(z) E = \frac{d}{dz}\left(\frac{1}{\mu(z)}\frac{dE}{dz}\right)$$

electric field

variable **permittivity**

variable **permeability**

Acoustic waves

$$-\omega^2 \frac{1}{\rho(z)c^2(z)} P = \frac{d}{dz}\left(\frac{1}{\rho(z)}\frac{dP}{dz}\right)$$

pressure

variable **velocity of sound**

variable **mass density**

Elastic longitudinal/shear waves

$$-\omega^2 \rho(z) u = \frac{d}{dz}\left(E(z)\frac{du}{dz}\right)$$

displacement

variable **mass density**

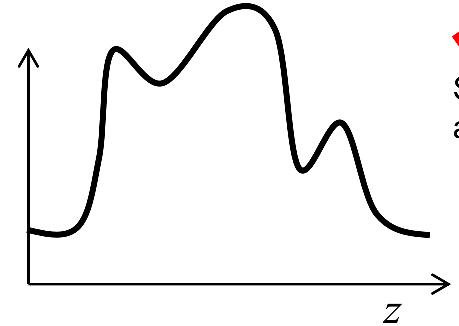
variable **modulus**

Electric transmission lines (tapered *LC* lines : ***$L(z)$, $C(z)$*** **)**

Ocean gravity waves, …

Foreword (5/5): Motivation and objectives

Graded profile

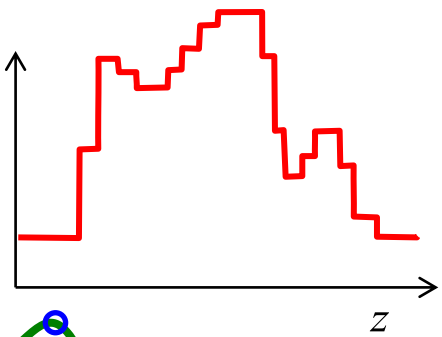


Standard approaches

1- The profile is one of known analytically solvable profiles (linear, power law, …)

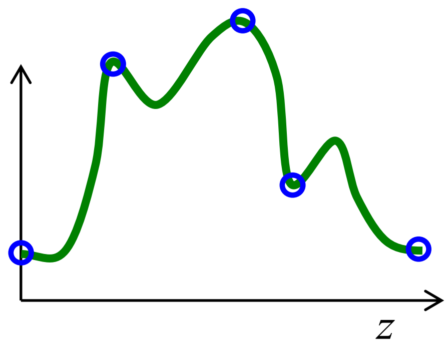
- exact solution
- limited flexibility
- special functions (CPU time ↗)

2- Staircase approximation
+ Analytical Transfer Matrix method (standard **quadrupole**)



- easy to implement
- approximate; constraint for good accuracy.

Proposed method



3- Piece-wise solution with :

- elementary **solvable profiles** with
- high flexibility
- elementary functions (CPU time ↘)

Heat equations for temperature and for heat flux

Hypotheses:
- 1D transfer
- Linear
- No heat sources
- Transient or steady periodic

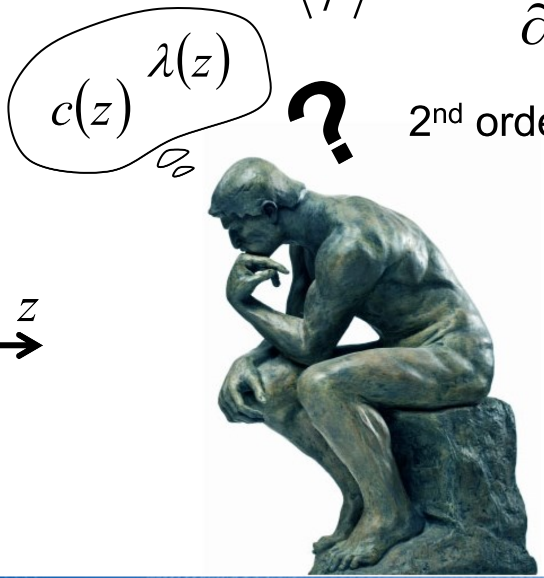
Energy-balance

$$\begin{cases} c(z)\dfrac{\partial T}{\partial t} = -\dfrac{\partial \varphi}{\partial z} \\ \varphi = -\lambda(z)\dfrac{\partial T}{\partial z} \end{cases}$$

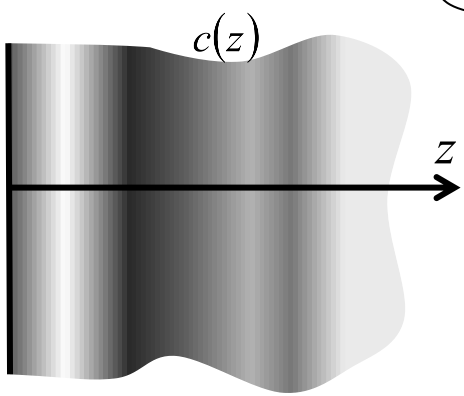
Fourier law

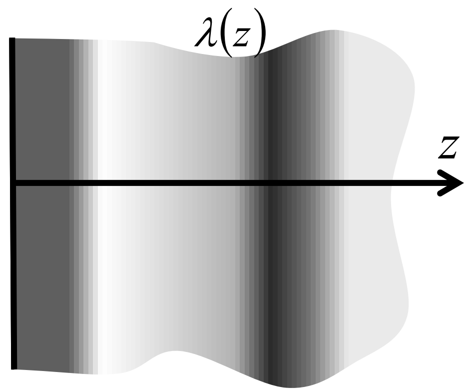
$$\langle T \rangle : \quad \frac{\partial T}{\partial t} = \frac{1}{c(z)}\frac{\partial}{\partial z}\left(\lambda(z)\frac{\partial T}{\partial z}\right)$$

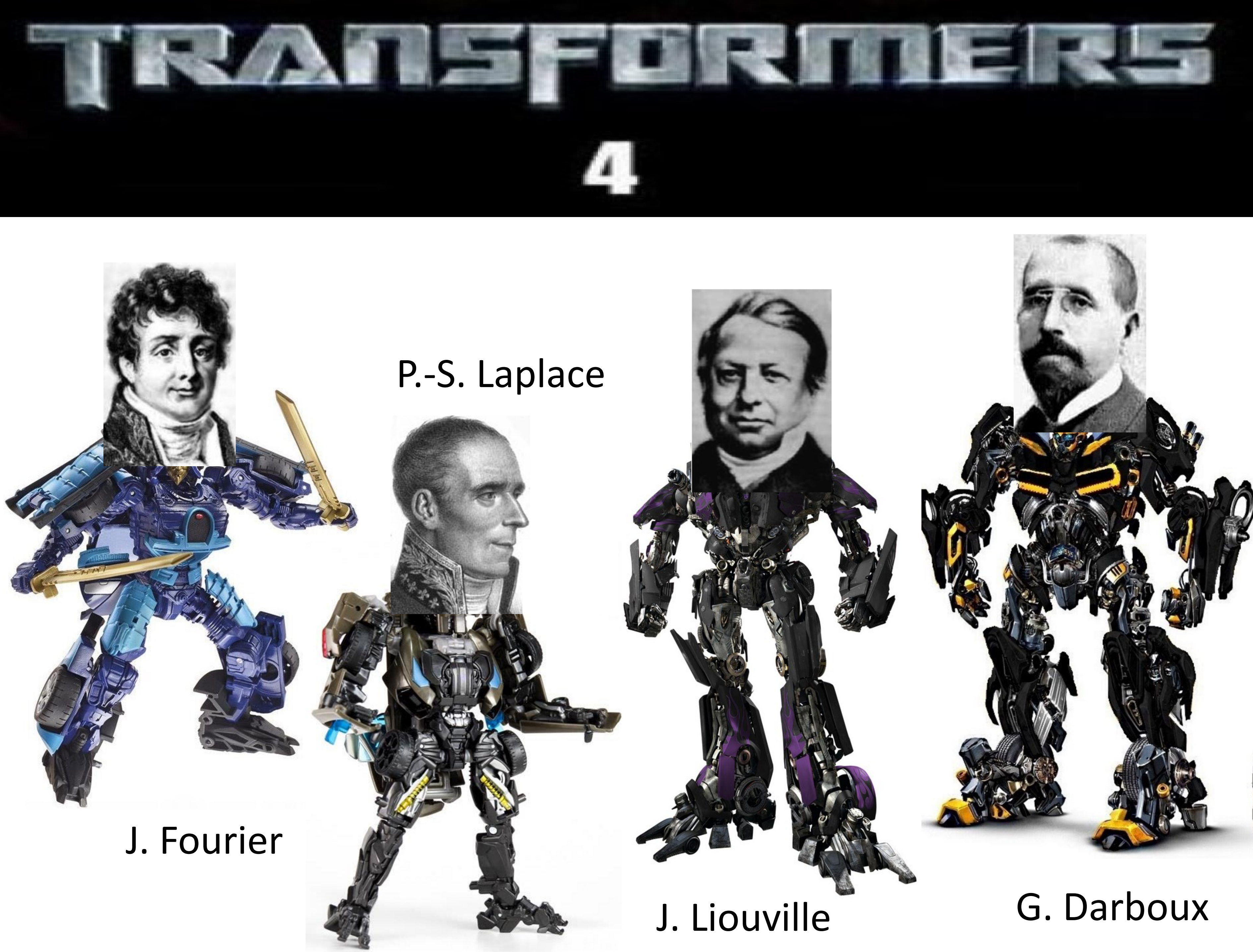
$$\langle \varphi \rangle : \quad \frac{\partial \varphi}{\partial t} = \lambda(z)\frac{\partial}{\partial z}\left(\frac{1}{c(z)}\frac{\partial \varphi}{\partial z}\right)$$



2nd order PDEs with **two variable coefficients**






TRANSFORMERS
4
P.-S. Laplace
J. Fourier
J. Liouville
G. Darboux

Laplace or Fourier transform

Elimination of the time-derivative
Multiplication by « p » variable

$$\langle T \rangle : \qquad p\theta = \frac{1}{c(z)}\frac{d}{dz}\left(\lambda(z)\frac{d\theta}{dz}\right)$$

$$\langle \varphi \rangle : \qquad p\phi = \lambda(z)\frac{d}{dz}\left(\frac{1}{c(z)}\frac{d\phi}{dz}\right)$$

p :

- Laplace variable (complex)
- Fourier variable $i\omega$ (pure imaginary)

2[nd] order ODEs with **two variable coefficients**

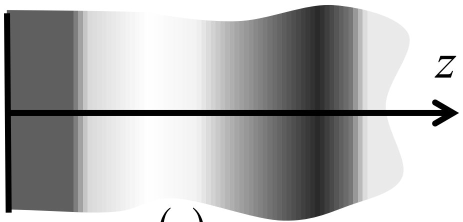
Liouville transformation (1897). First step

First step : a **change of the independent-variable:**

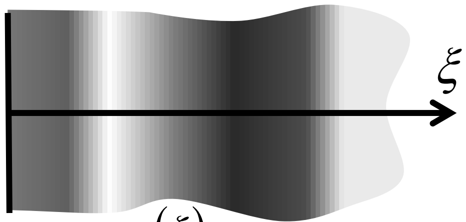
$$z \to \xi(z) := \int_0^z \frac{du}{\sqrt{a(u)}}$$

Transformation involving the **diffusivity** profile: $a(z) := \lambda(z)/c(z)$

Physical coordinate z → **Square-root of diffusion time (SRDT)** ξ



$a(z)$



$a(\xi)$

$\langle T \rangle$: $\quad p\theta = b^{-1}(b\theta')'$

$\langle \varphi \rangle$: $\quad p\phi = b(b^{-1}\phi')'$

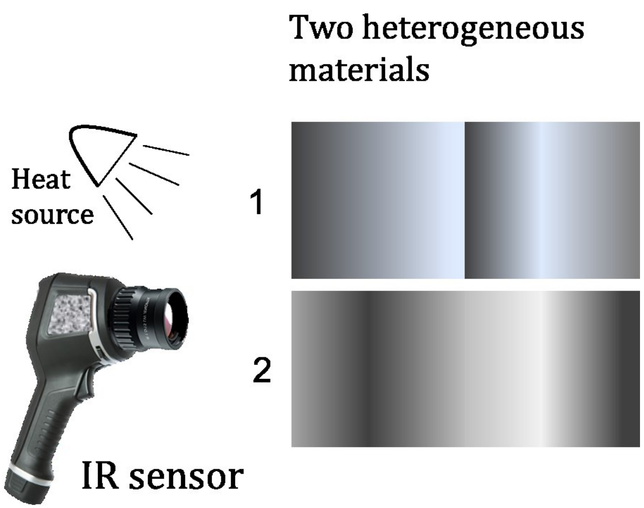
2nd order ODEs with **only one variable coefficient:**

Effusivity $\quad b(\xi) := \sqrt{\lambda(\xi)c(\xi)}$

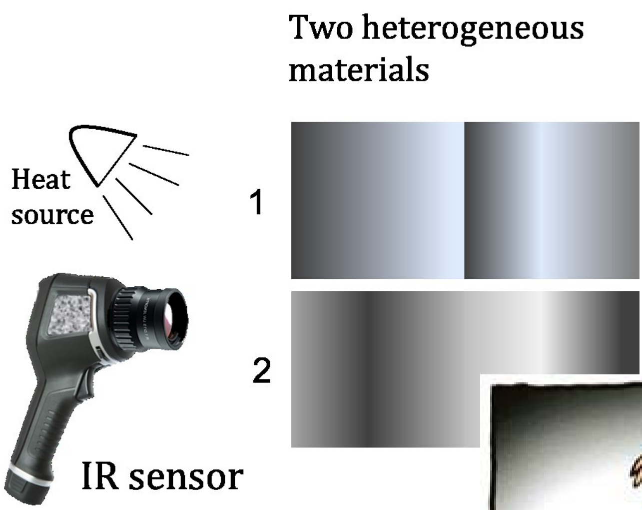
⇒

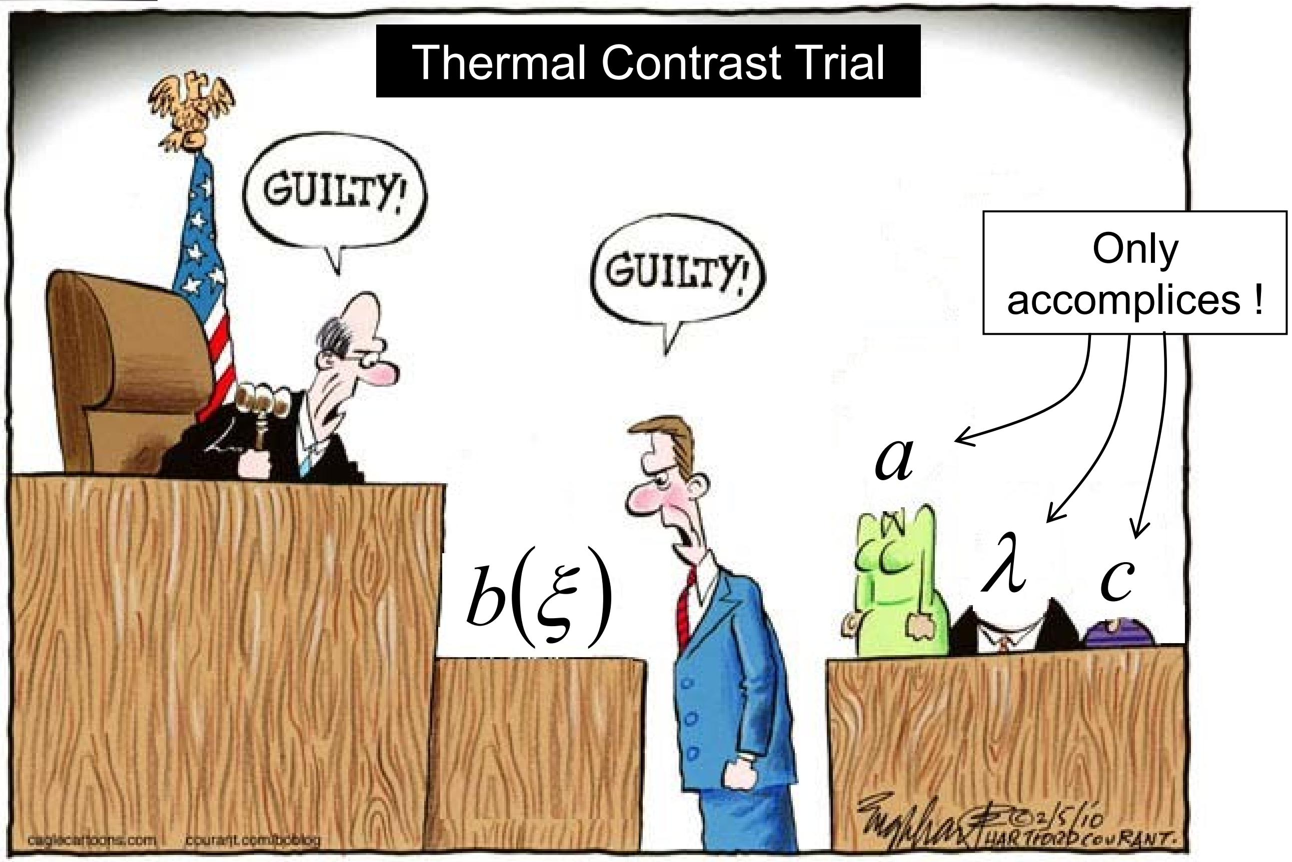
- **Outstanding importance** of the **effusivity profile**
- $b(\xi)$ is **solvable** ⟷ $b^{-1}(\xi)$ is **solvable**

Who is responsible for the thermal contrast ?



Who is responsible for the thermal contrast ?





The **effusivity profile**

$$b(\xi)$$

is the brain of the band !

I apologize to B. Englehart for the misappropriation of his cartoon …

Liouville transformation (1897). Second step

Second step : a **change of the dependent-variable:**

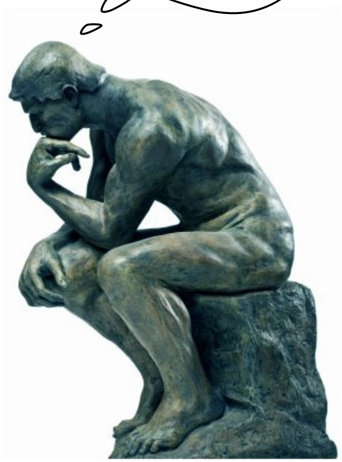
$$\begin{cases} \langle T \rangle : & \theta \to \psi := \theta\, b^{+1/2}(\xi) \\ \langle \varphi \rangle : & \phi \to \psi := \phi\, b^{-1/2}(\xi) \end{cases}$$

In both cases we obtain a **Stationary Schrödinger Equation** (SSE)

$$\psi'' = (V + p)\psi$$

"**potential**" $V(\xi) := \dfrac{s''}{s}$ **reduced 2nd derivative**

Reduced 2nd derivative. So what ?



The "**metaproperty**" $s(\xi)$ is defined by: $s := \begin{cases} b^{+1/2} & ;\langle T \rangle - form \\ b^{-1/2} & ;\langle \varphi \rangle - form \end{cases}$

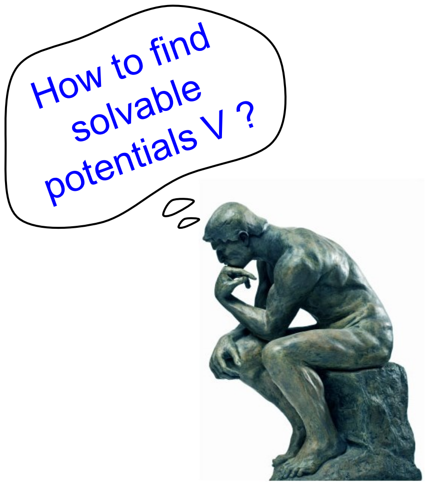
The TRICK: cast the SSE equation into **two homologous** SSEs

Recast the definition of the "potential" $V(\xi) := s'' / s \;\Rightarrow\; s'' = V(\xi)s$

$$\psi'' = \left(V(\xi) + p\right)\psi$$
$$s'' = V(\xi)s$$

- the **thermal field** ψ
- the **meta-property** s

satisfy two **homologous** Schrödinger equations (i.e. with the **same potential**)



Constant potential → « Fundamental solutions »

$$\psi'' = \left(V(\xi) + p\right)\psi$$
$$s'' = V(\xi)s$$

$$\langle T \rangle - form: \quad s = b^{+1/2} \quad ; \psi = \theta b^{+1/2}$$
$$\langle \varphi \rangle - form: \quad s = b^{-1/2} \quad ; \psi = \varphi b^{-1/2}$$

$V(\xi) = \beta = 0$ → **Linear** solutions for
$V(\xi) = \beta > 0$ → **Hyperbolic** solutions for
$V(\xi) = \beta < 0$ → **Trigonometric** solutions for

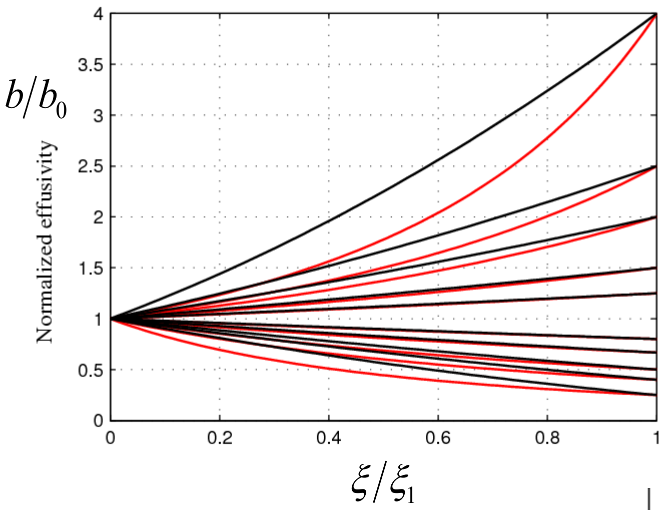
} $b^{\pm 1/2}(\xi)$

Solution for the field function:

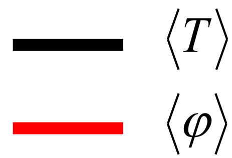
$$\psi(\xi, p) \propto \begin{bmatrix} \cosh\left(\sqrt{p+\beta}\,\xi\right) \\ \sinh\left(\sqrt{p+\beta}\,\xi\right) \end{bmatrix}$$

Generalization of the particular case with constant diffusivity:
Sutradhar A. et al., Comput. Meth. Appl. Mech. Engrg. (2004)

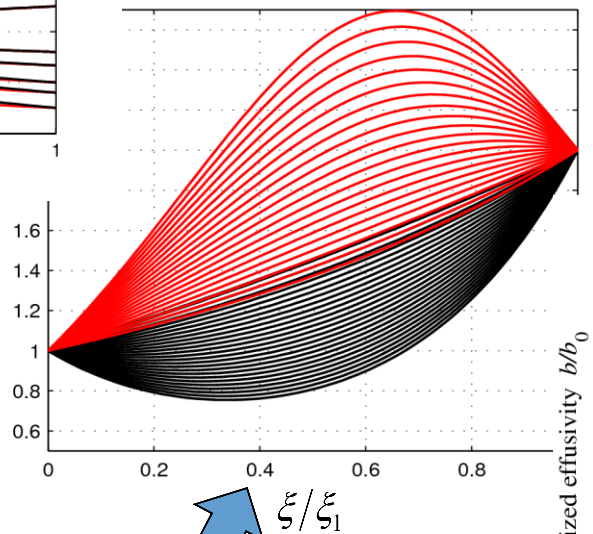
A few “fundamental profiles” of the effusivity



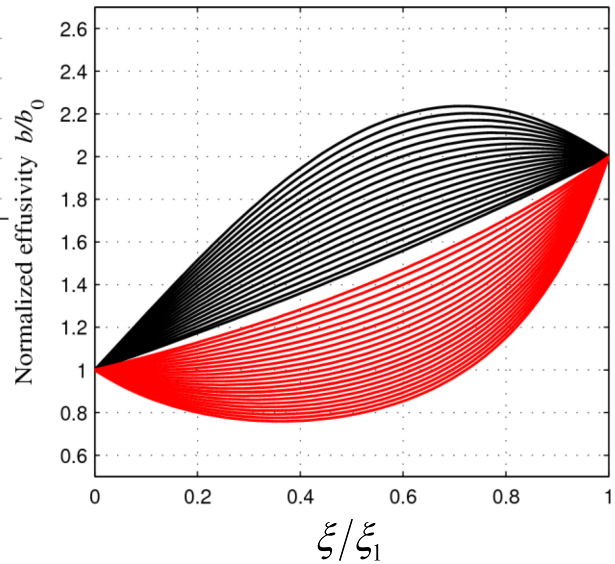
“**Linear**” profiles



“**Hyperbolic**” profiles



“**Trigonometric**” profiles



Different values of b_1/b_0

Essentially **concave or convex shape**

$b_1/b_0 = 2$

and different values for the “potential”

Darboux transformation (DT)
« Un curieux théorème d'analyse » (1882, 1889)

$$\psi'' = \left(V_n(\xi) + p\right)\psi$$

Given a **solvable** SSE

$$\psi'' = \left(V_{n+1}(\xi) + p\right)\psi$$

Construction of another **solvable** SSE with a **new potential function** $V_{n+1}(\xi)$

- A **cascade** procedure for finding **closed-form** analytical solutions **for both** :
  - Effusivity profile
  - Temperature/heat-flux distribution

  → joint ***Property & Field Darboux Transformation*** (**PROFIDT**)

- Up to **2 additional parameters** per step

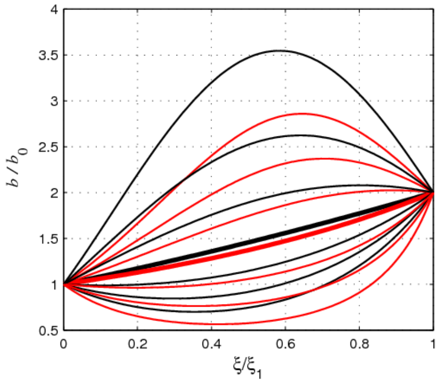
  → profiles with **increasingly complex shape**

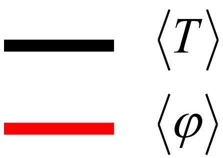
- When starting with a **constant seed-potential**

  → all solutions involve only **elementary** functions

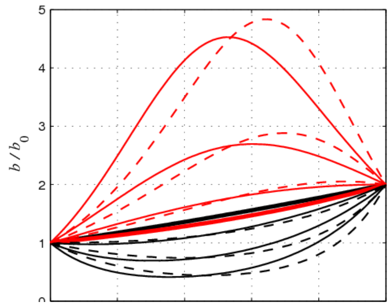
PROFIDT → plenty of new solvable profiles

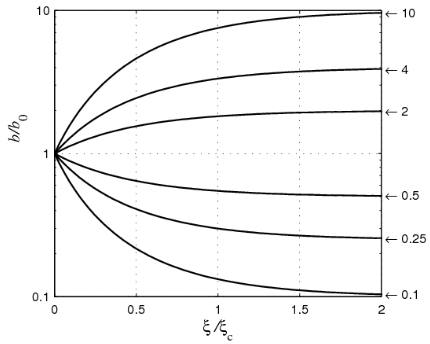
- **Fundamental** solutions (constant potential)

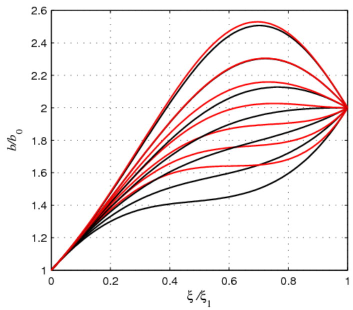


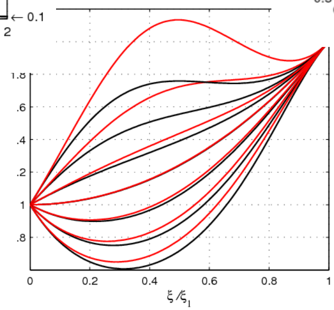


- **One PROFIDT**

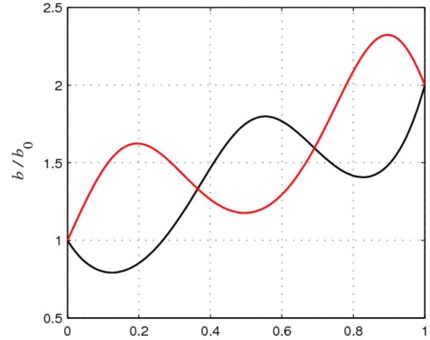


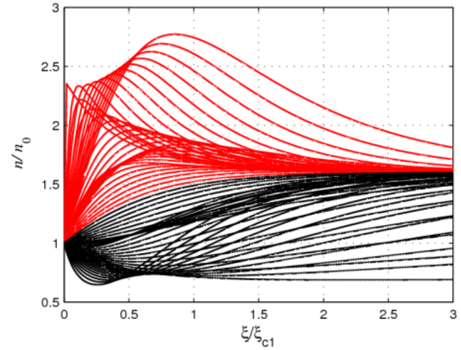






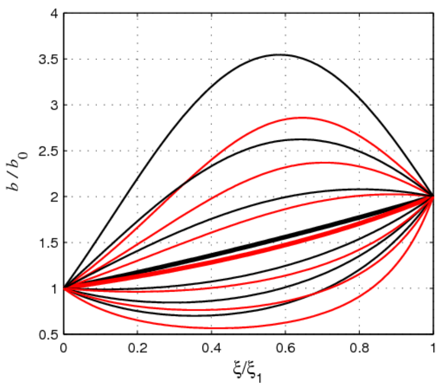
- **Two PROFIDTs**



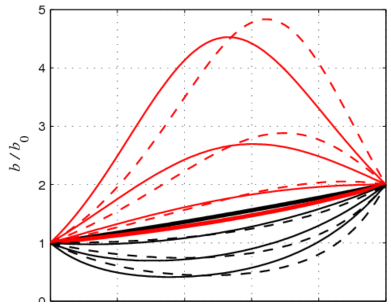


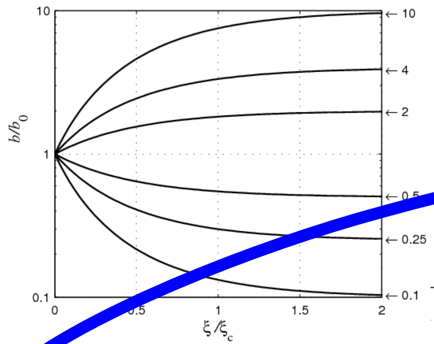
PROFIDT → plenty of new solvable profiles

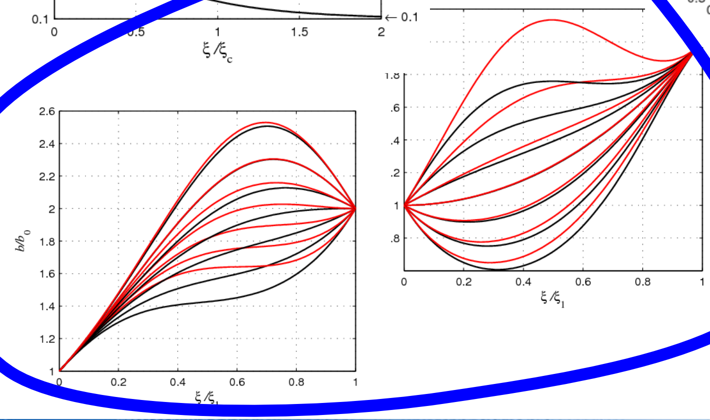
- **Fundamental** solutions (constant potential)



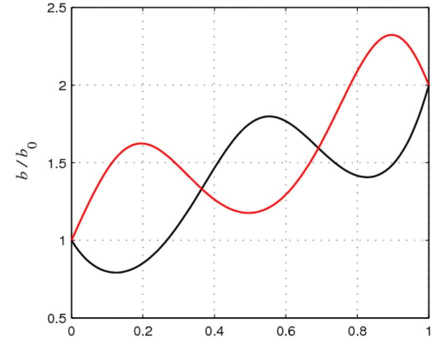
- **One PROFIDT**

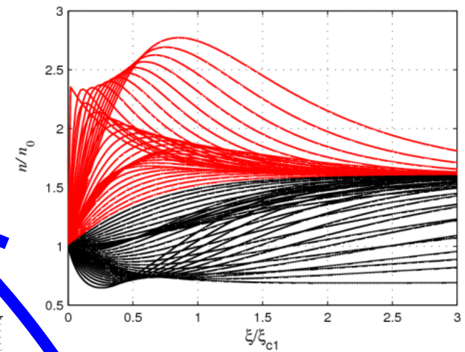






- **Two PROFIDTs**

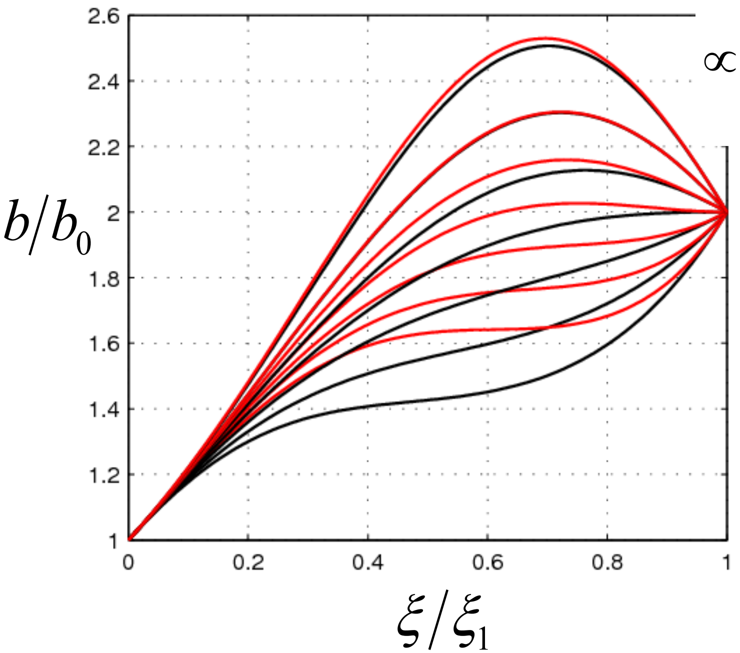




$\langle T \rangle$ (black)

$\langle \varphi \rangle$ (red)

One single PROFIDT with seed potential $V_0(\xi) = \xi_c^{-2} > 0$ and $p_1 = 0$. Profiles of $\mathrm{sech}(\hat{\xi})$-type ([sεk ksi hæt])



$$\propto \left[\frac{\mathrm{sech}(\hat{\xi})}{\sinh(\hat{\xi}) + \hat{\xi}\,\mathrm{sech}(\hat{\xi})} \right]$$

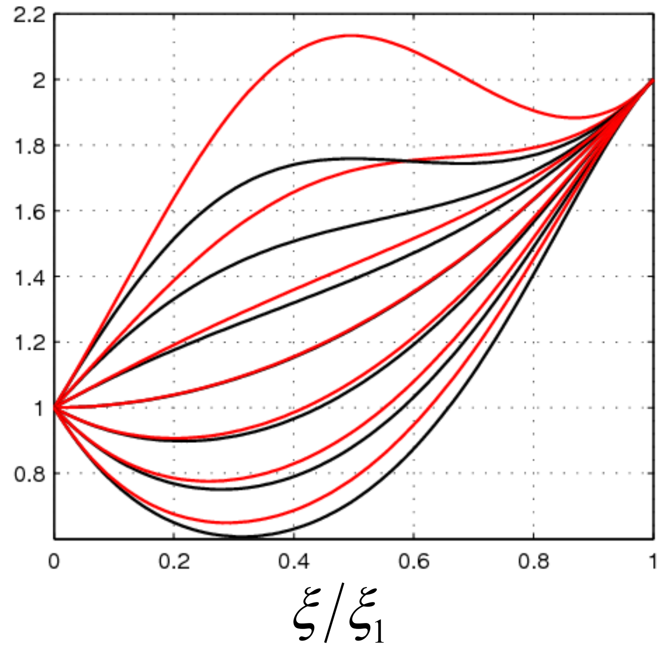
$$\hat{\xi} := \xi/\xi_c + \tau$$

$$\mathrm{sech} := 1/\cosh$$

Hyperbolic secant function

Black line: $\langle T \rangle$

Red line: $\langle \varphi \rangle$



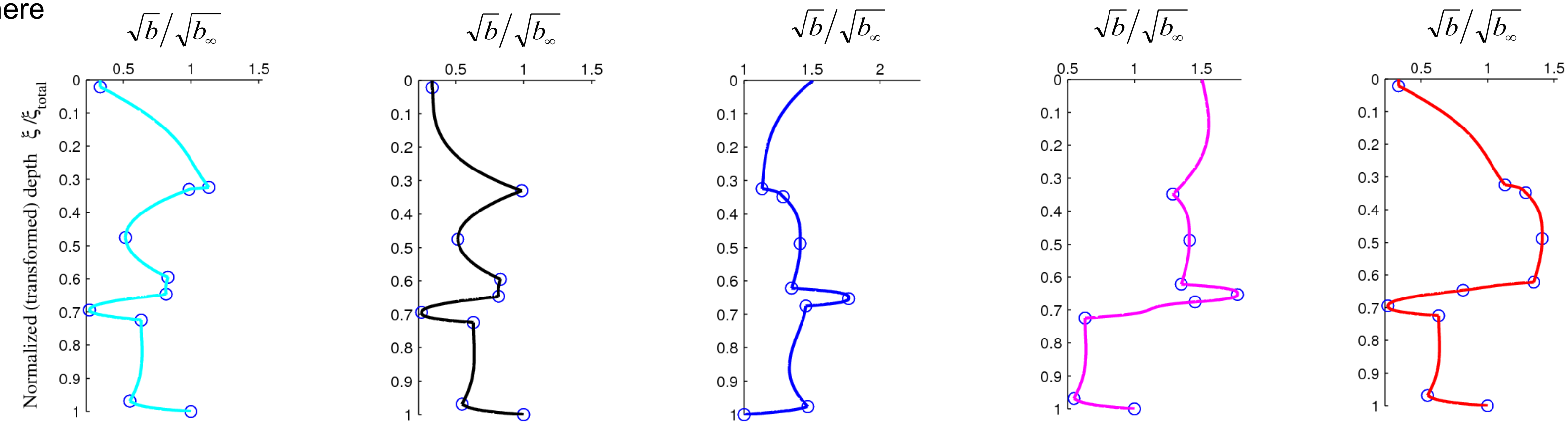
- **Two sub-classes** of profiles : $\langle T \rangle$ -form and $\langle \varphi \rangle$ -form
- **Relatively simple quadrupole (only exp. functions)**
- **4 adjustable parameters** ξ_c, τ and two multiplicative factors
- **Absolutely flexible** : can accomodate any specification regarding { two end-values / two end-slopes

Elementary bricks to perform **spline interpolation** (like cubic polynomials) → **new concept of solvable splines**

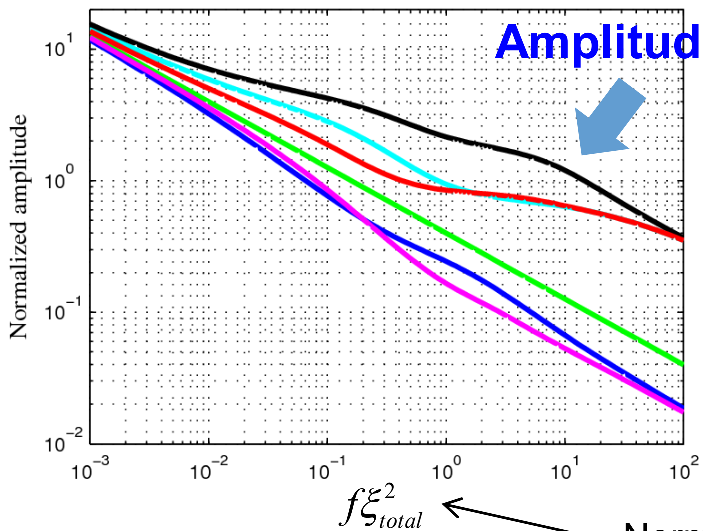
And now, a « light » example of synthetic profiles with the corresponding temperature responses

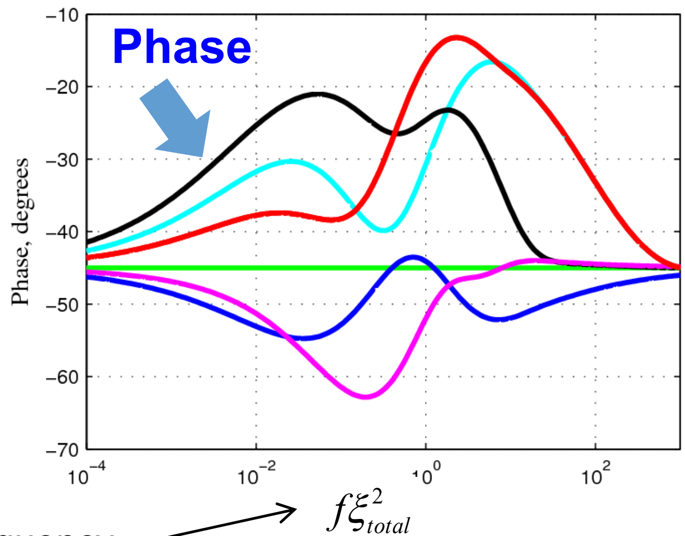
Photothermal experiment from here

Five synthetic profiles of **thermal effusivity (8 to 10** $\mathrm{sech}\left(\hat{\xi}\right)$ **elements)**



Spectra of the **photothermal response** (modulated surface **temperature**)





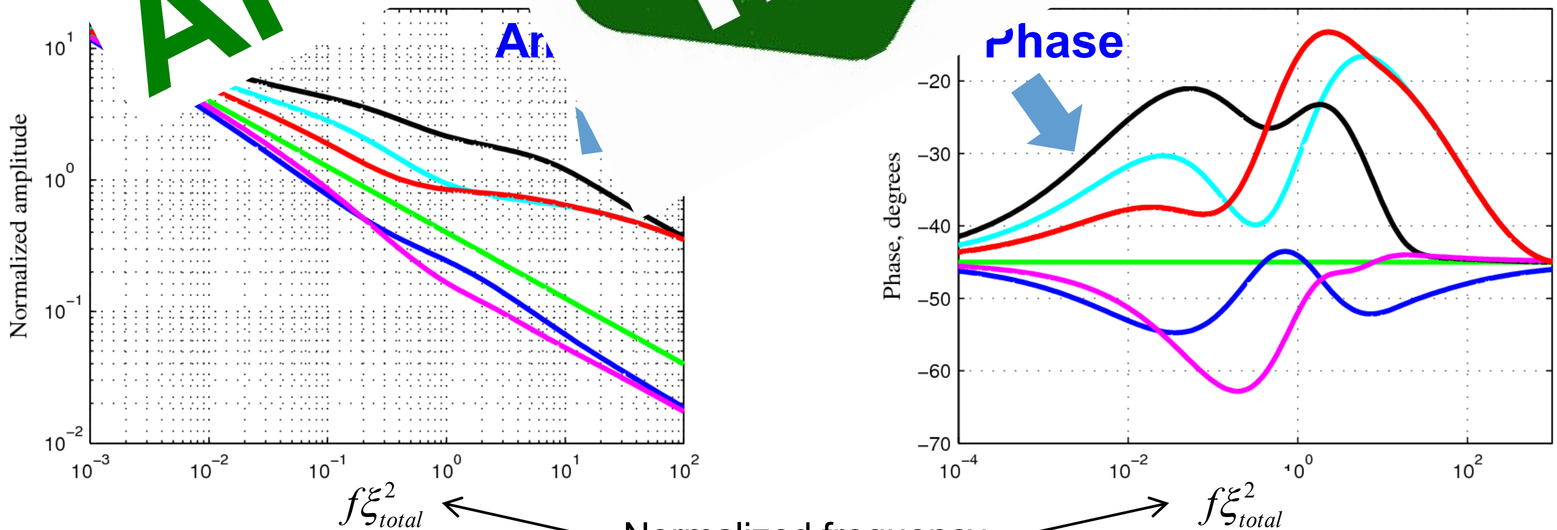
Normalized frequency

And now, a « light » example of synthetic profiles with the corresponding temperature responses

Photothermal experiment from here

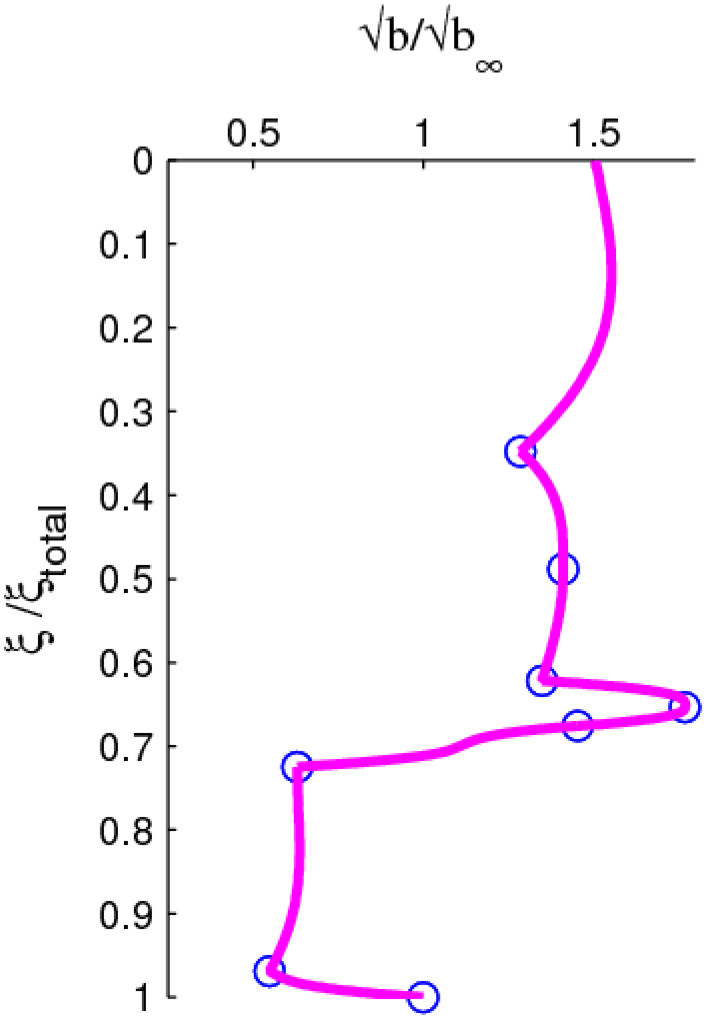
Synthetic profile… …sivity (8 to 1… …ments)

…temperature)



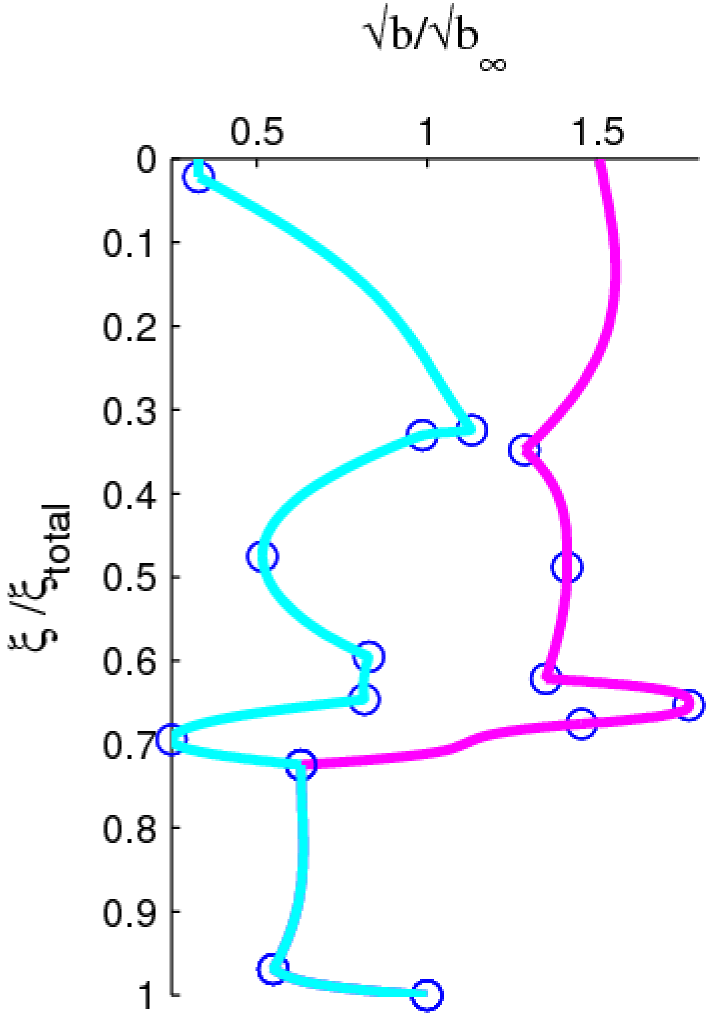
Normalized frequency

The hidden motivation…



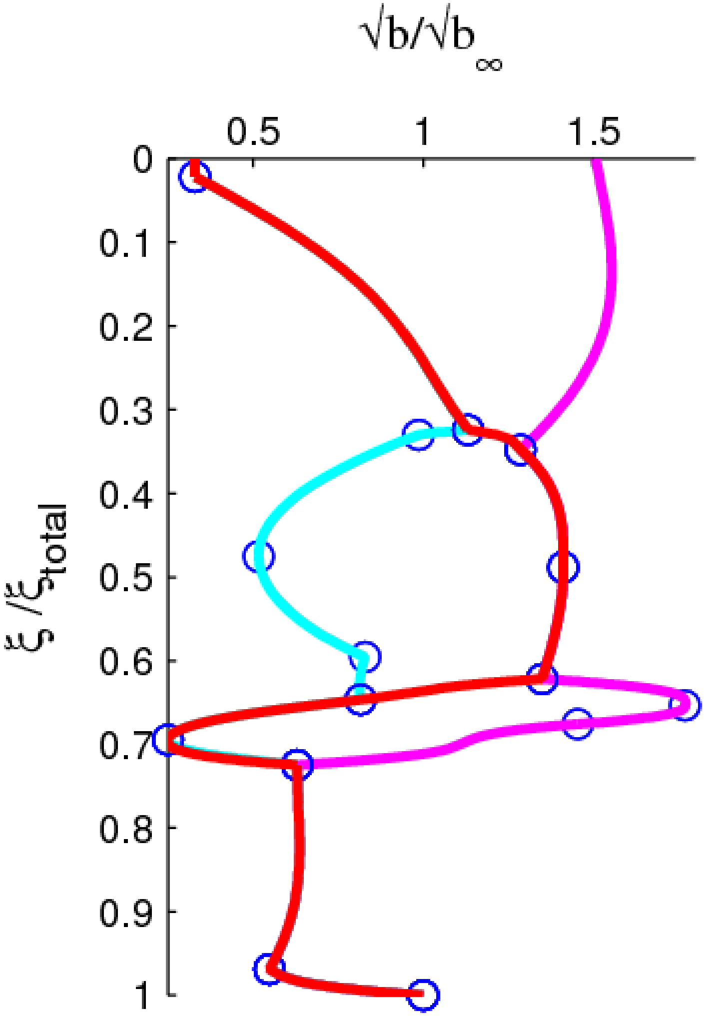
By superimposing all these synthetic profiles…

The hidden motivation…



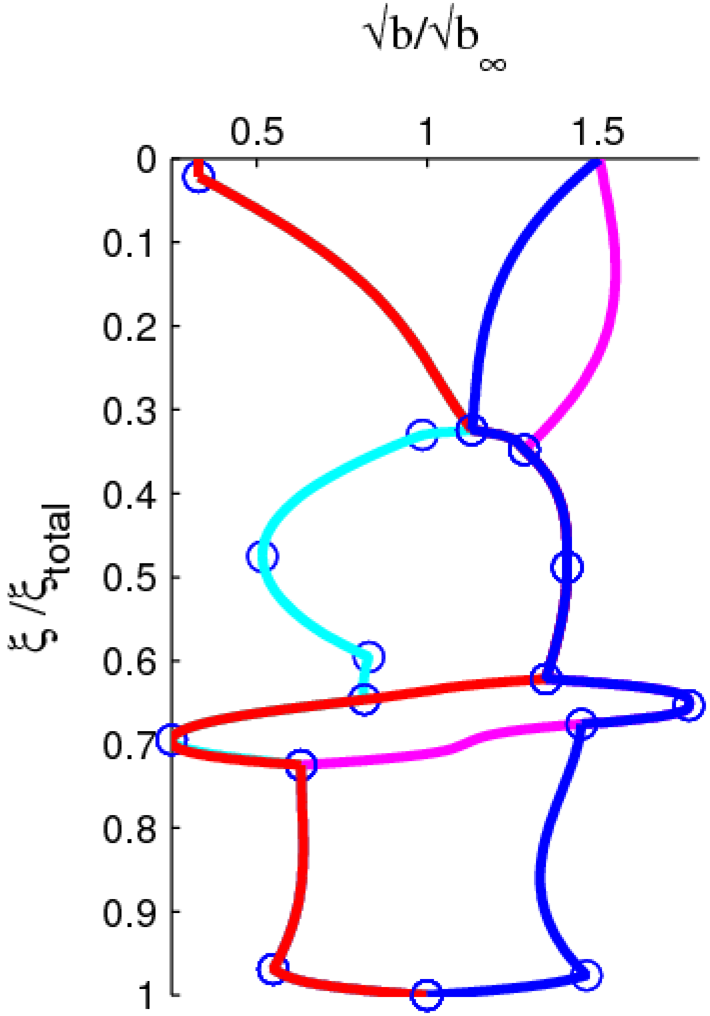
By superimposing all these synthetic profiles…

The hidden motivation…



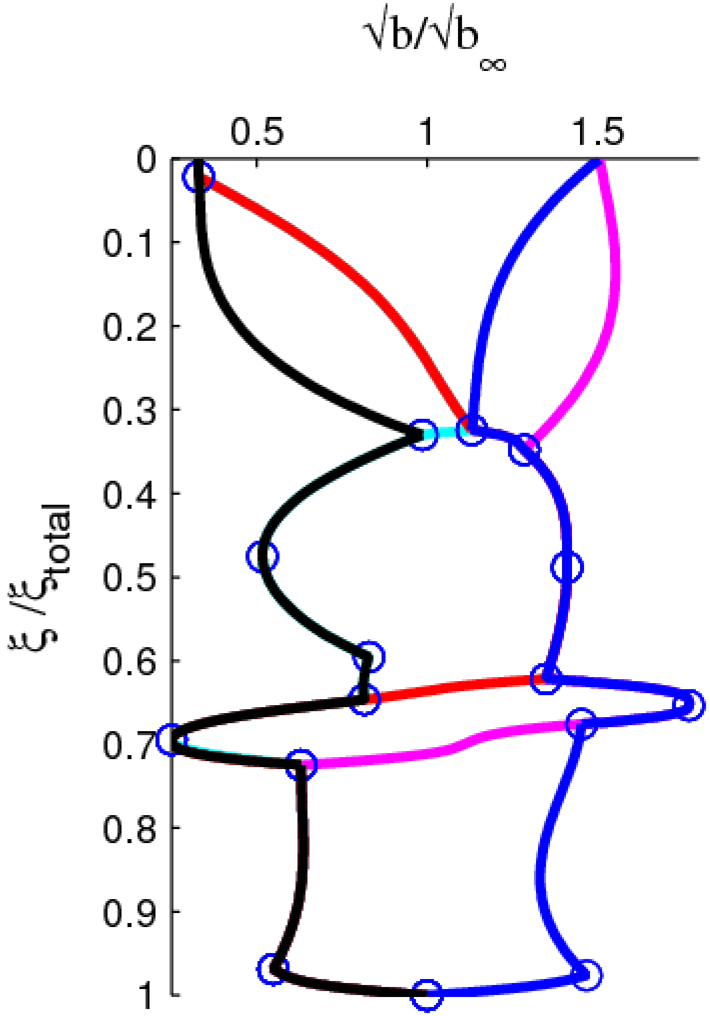
By superimposing all these synthetic profiles…

The hidden motivation…



By superimposing all these synthetic profiles…

Examples of synthetic graded profiles

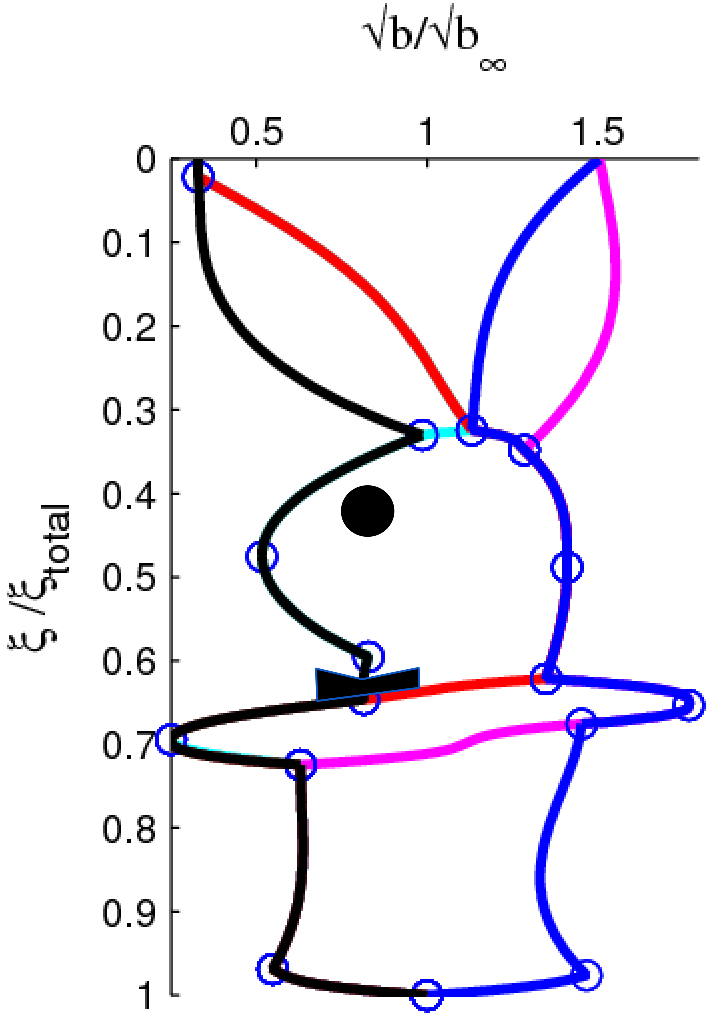


By superimposing all these synthetic profiles…

we come to a representation that :

- illustrates the versatility of the $\mathrm{sech}\left(\hat{\xi}\right)$ profiles

Examples of synthetic graded profiles



By superimposing all these synthetic profiles…

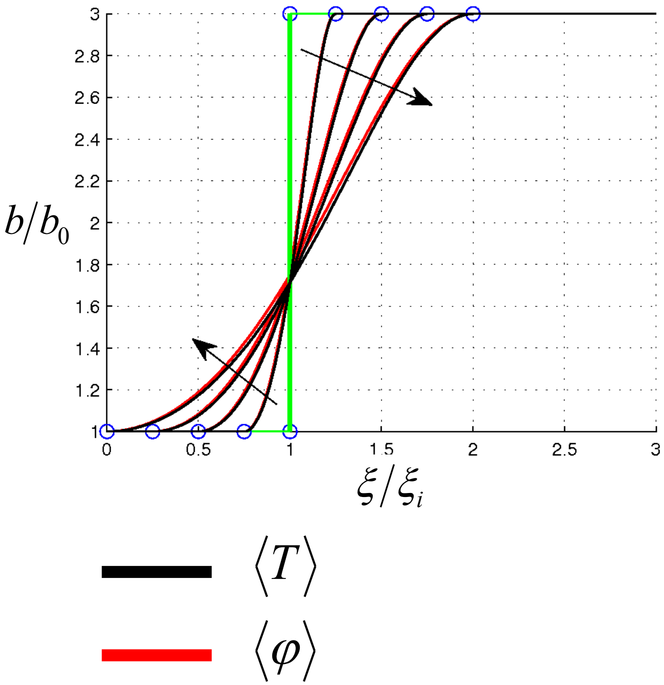
we come to a representation that :

- illustrates the versatility of the $\mathrm{sech}(\hat{\xi})$ profiles
- will allow you to easily memorize the name of these **[sɛksi hæt]** profiles

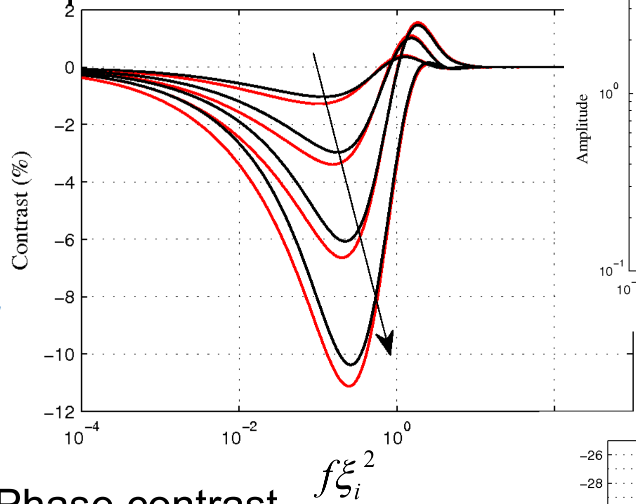
And now, a « serious » example : diffuse interfaces

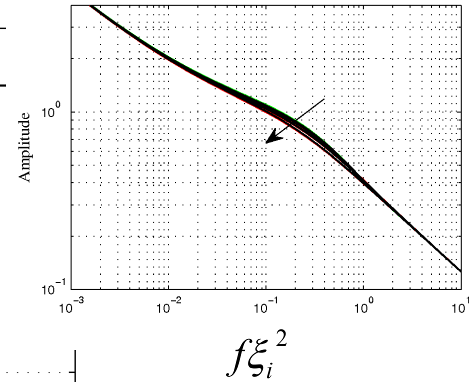
Sharp interface vs. **diffuse** interface

progressively
smoother interface

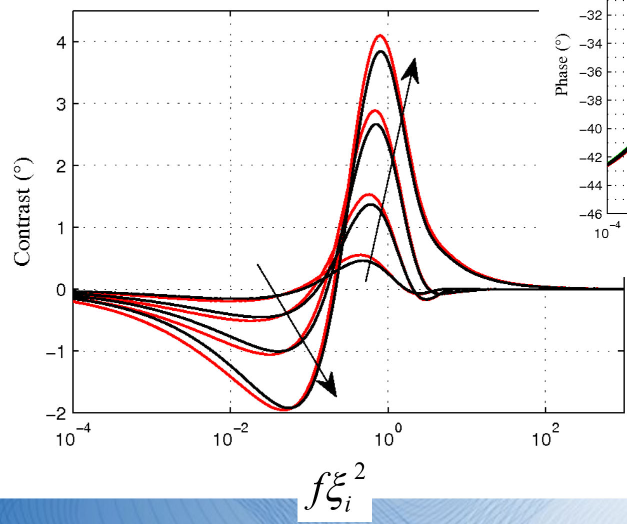


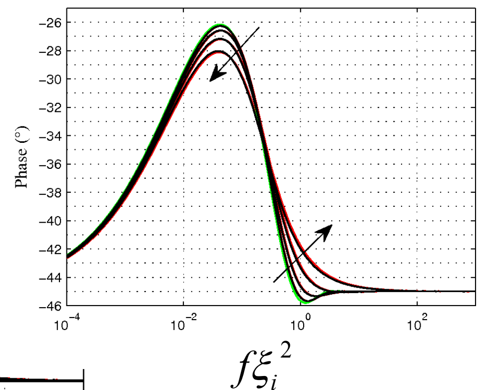
Amplitude contrast





Phase contrast





Modeling of the dispersion of pollutants in the atmosphere

$$U_x(z)\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C}{\partial z}\right)$$

Essential parameter : the **« effective inertia » of the atmosphere** (with respect to contamination):

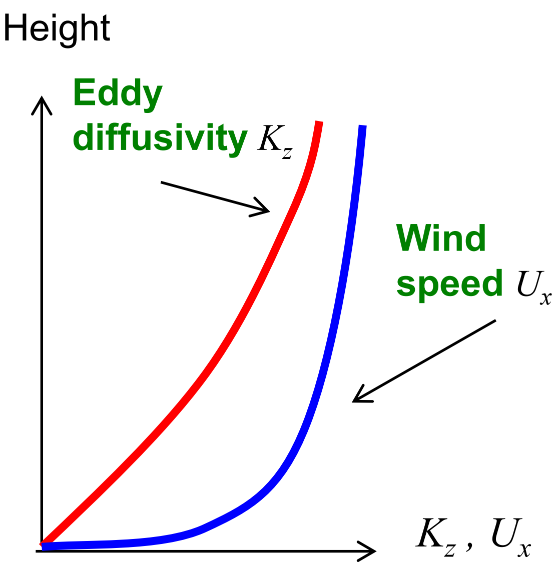
$$b := \sqrt{U_x(z)K_z(z)}$$

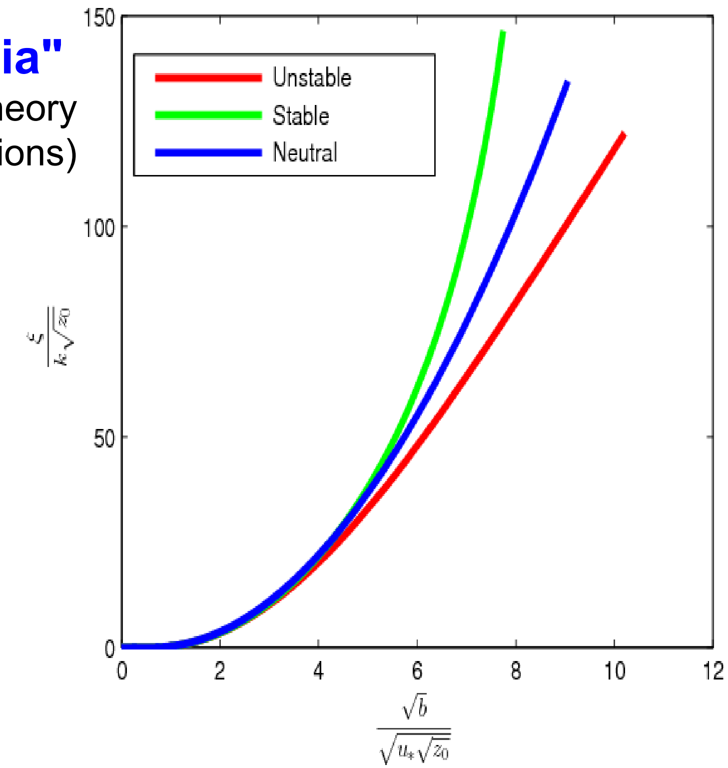
New independent variable:

$$\xi := \int_0^z \frac{\sqrt{U_x(z)}dz}{\sqrt{K_z(z)}}$$

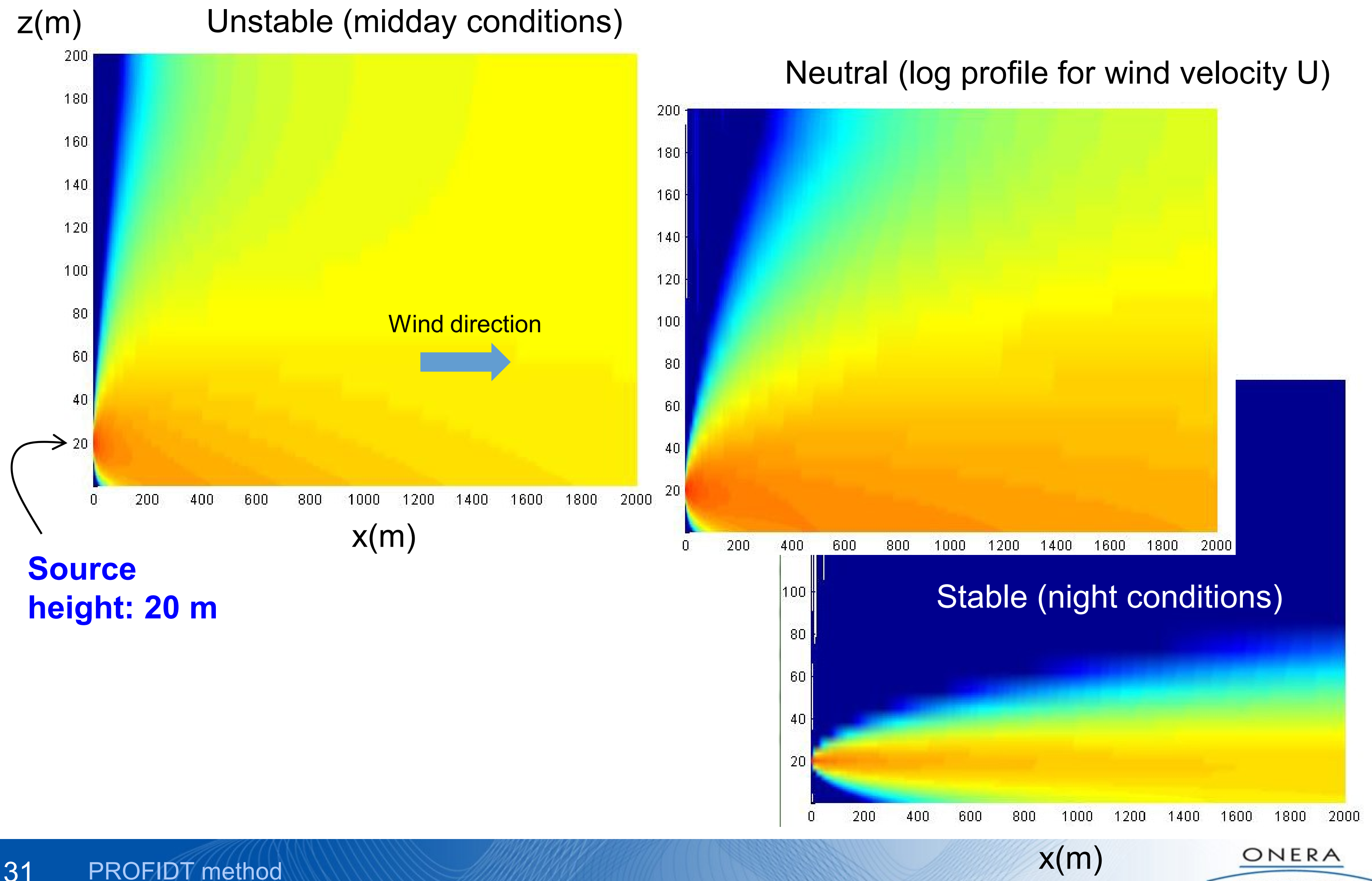
"Vertical" profiles of "inertia"

Monin-Obukhov similarity theory (Businger relations)





x-z distribution of pollutant concentration depending on the atmosphere stability

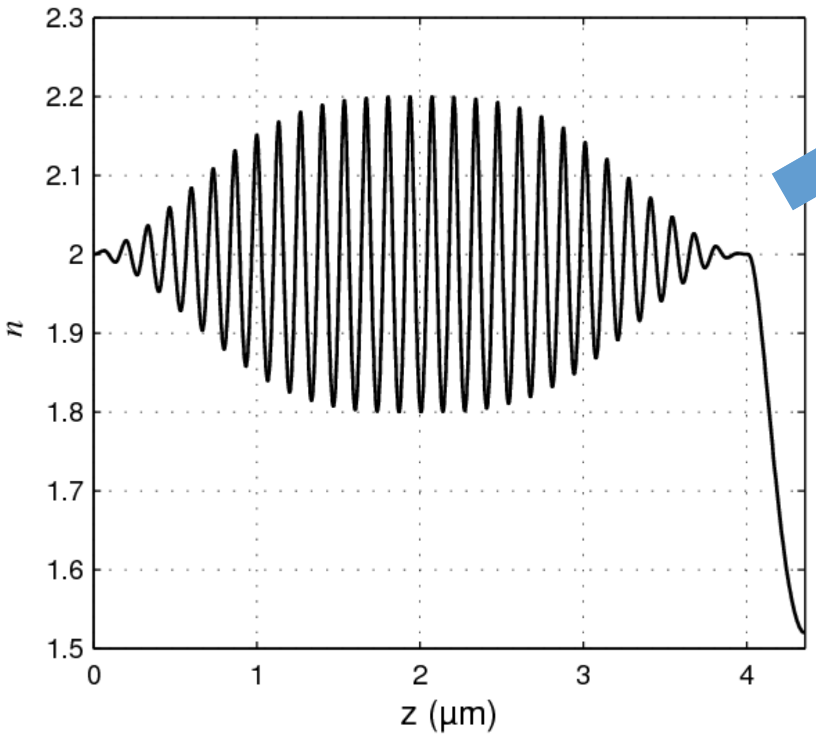


Applications in optics: filter design (dielectric thin films)

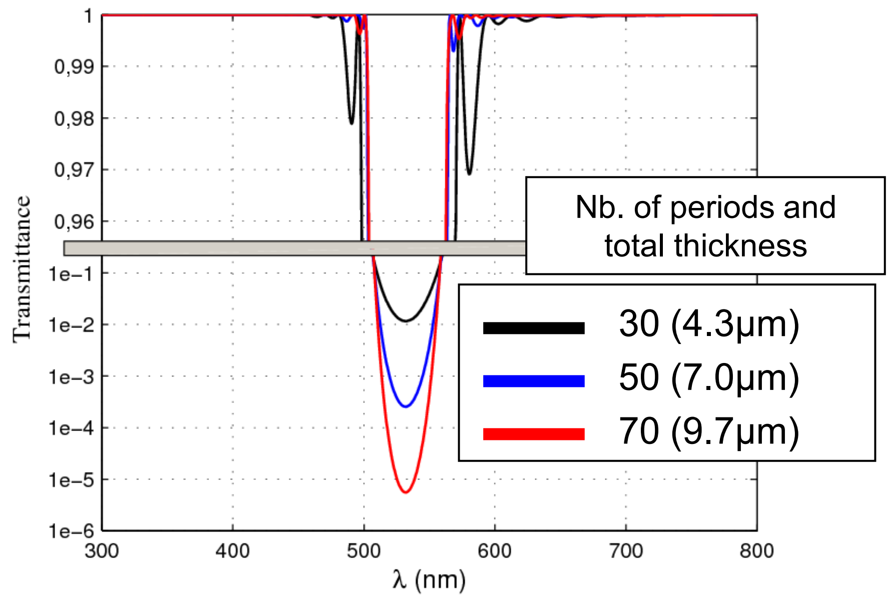
Rugate profile obtained by stitching **60** $\mathrm{sech}(\hat{\xi})$-type profiles of <E>-form (30 periods of 266nm optical thickness)

+ sinus-square **apodisation**

+ **matching layer** with 600nm optical thickness from n_0 =2 down to n_s =1.52 (substrate)



Transmittance spectrum of the notch filter



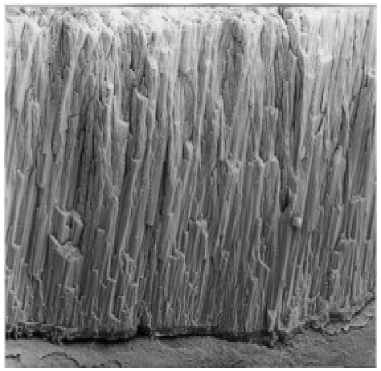
Only one transfer matrix per alternance (no need for finer discretisation)

Other applications : chirped mirrors (fs lasers) Bragg filters, photonic crystals, matching layers, etc…

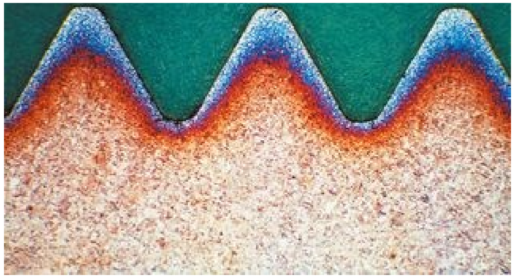
Thermal depth-profiling

Examples of « materials » with **graded properties**

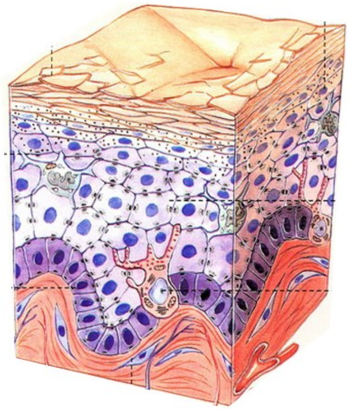
Soil



SEM of Thermal Barrier Coating



Case-hardened steel



Skin

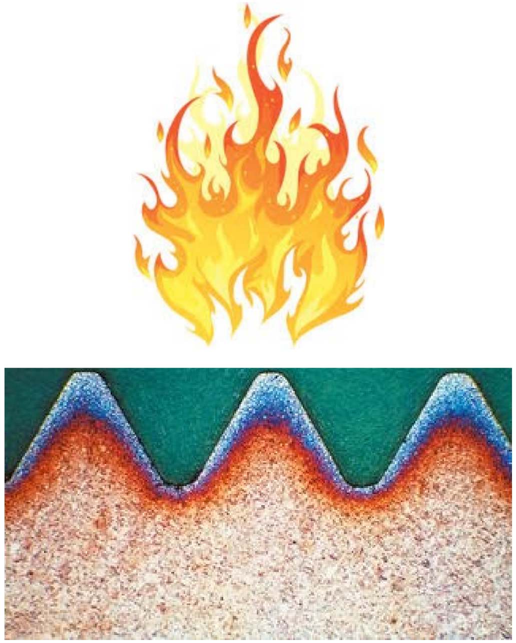
different nature and scales !

Thermal depth-profiling. Typical procedure

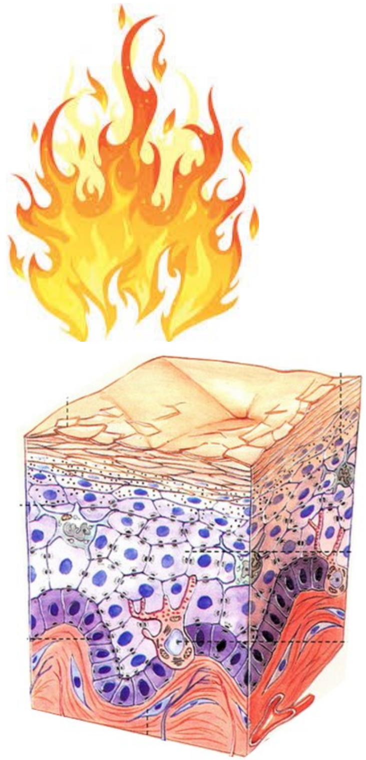
1- heat the surface (pulse or modulated)

Soil

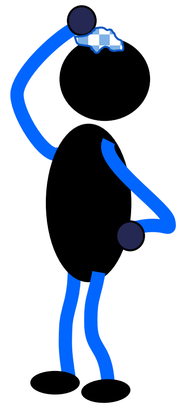
SEM of Thermal Barrier Coating



Case-hardened steel



Skin

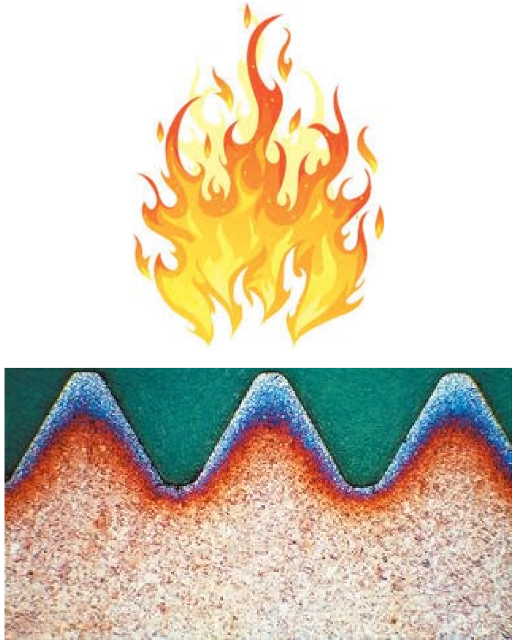


Thermal depth-profiling. Typical procedure

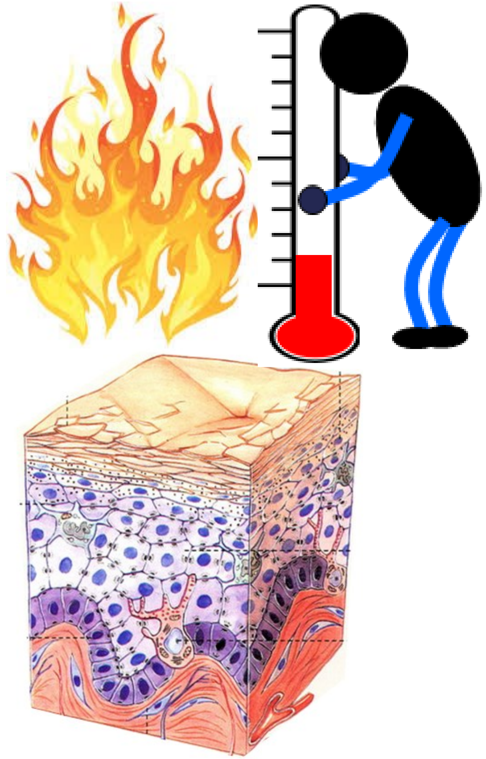
2- measure the temperature response (while heating or just after)

Soil

SEM of Thermal Barrier Coating



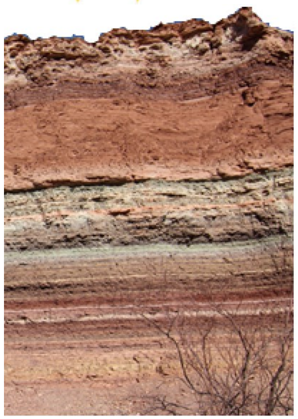
Case-hardened steel



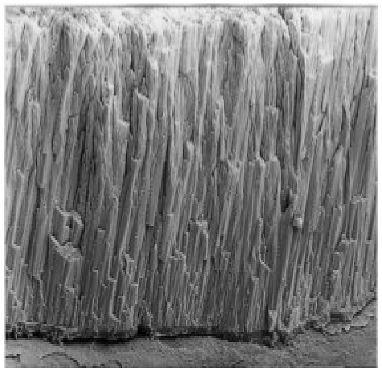
Skin

Thermal depth-profiling. Typical procedure

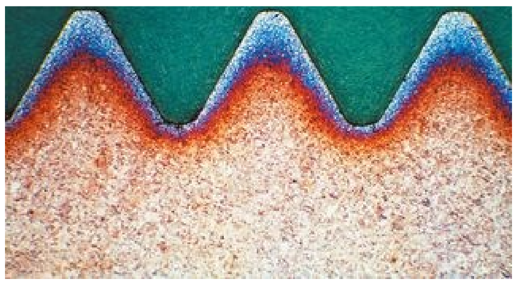
3- (stop heating and) process the data for inversion



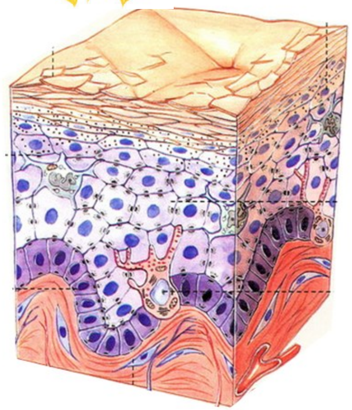
Soil



SEM of Thermal Barrier Coating



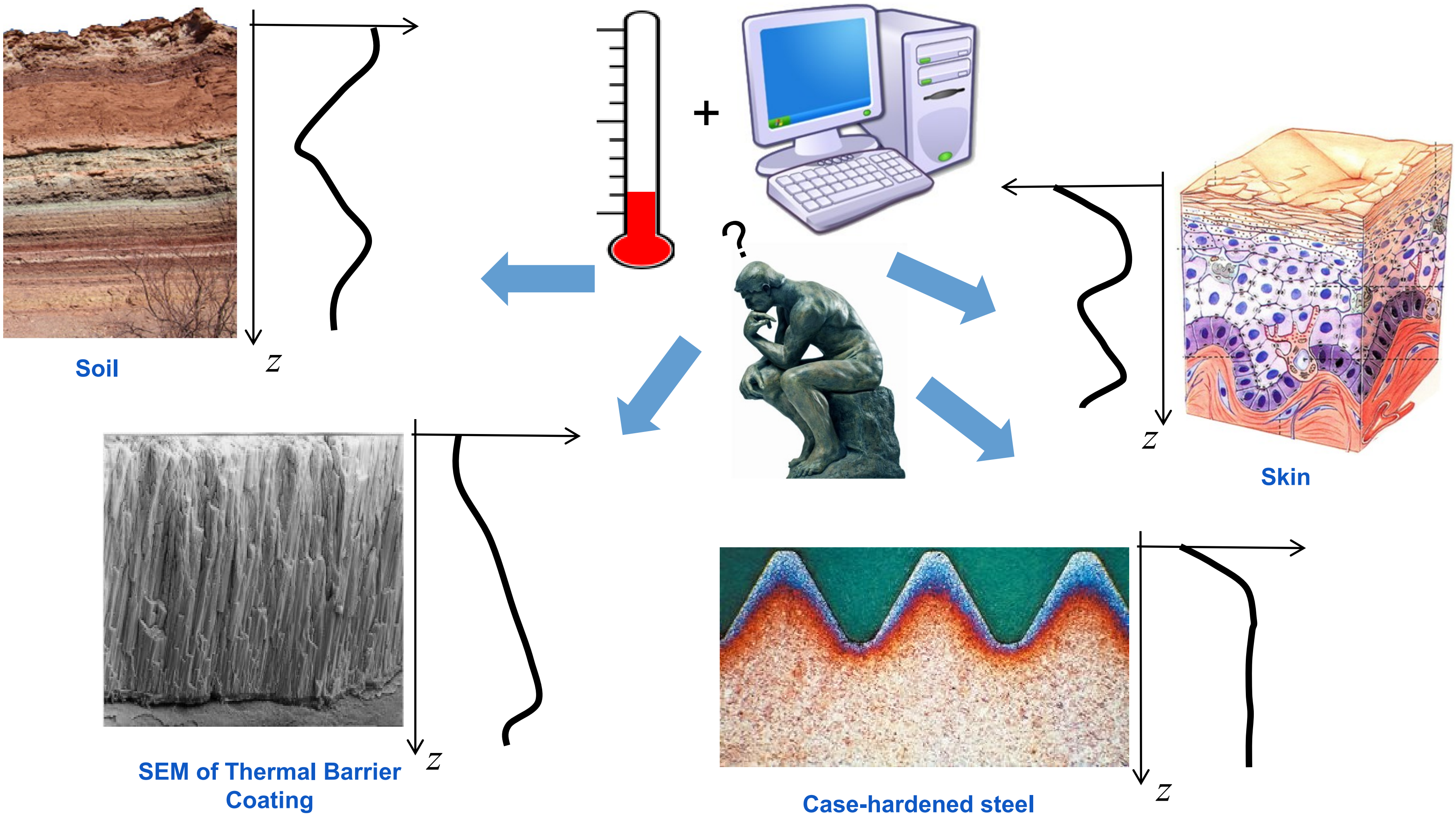
Case-hardened steel



Skin

Thermal depth-profiling. Typical procedure

4- identify the profile of the thermal property (…*which one* ?)



Inversion principle to evaluate the effusivity profile

1- **Minimize the mismatch** between the **experimental data** and the **theoretical data** as given by a **model with continuous parameters**

Cost function:

difference in temperature: $$F = \sum_{i=1}^{n} \left(T_{\text{th}}(t_i) - T_{\text{exp}}(t_i) \right)^2$$

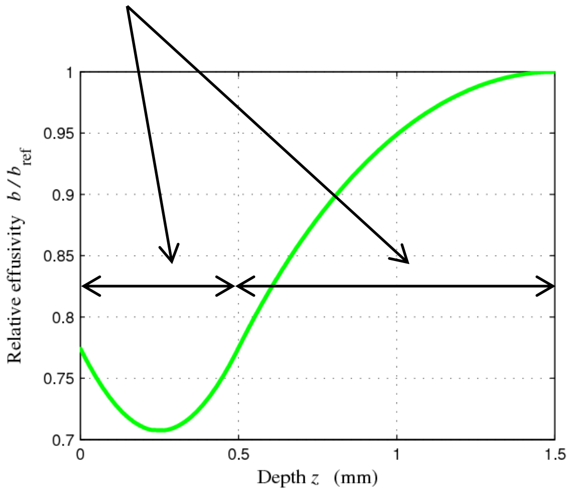
difference in *apparent effusivity*: $$F = \sum_{i=1}^{n} \left(\frac{1}{\sqrt{\pi t_i}\, T_{\text{th}}(t_i)} - \frac{1}{\sqrt{\pi t_i}\, T_{\text{exp}}(t_i)} \right)^2$$

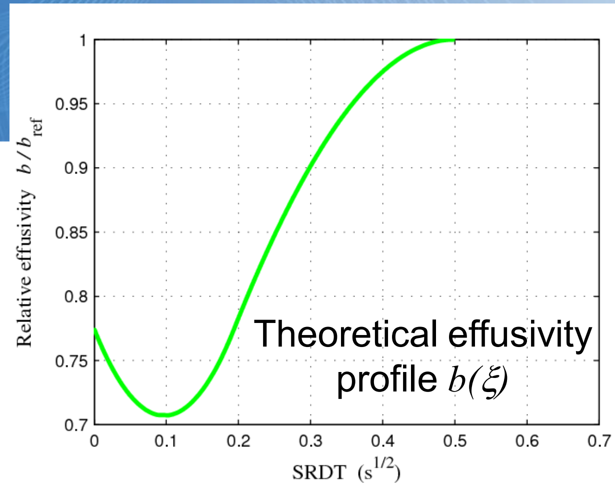
2- **Add as many** $\operatorname{sech}(\hat{\xi})$**-type profiles as necessary** to reduce residues to an acceptable level (i.e. stop as soon as all non-stochastic features have disappeared)

= **parsimonious regularization**

Inversion. Synthetic data

Theoretical effusivity profile $b(z)$: from a conductivity profile build with two quadratic polynomials (ρC assumed constant)



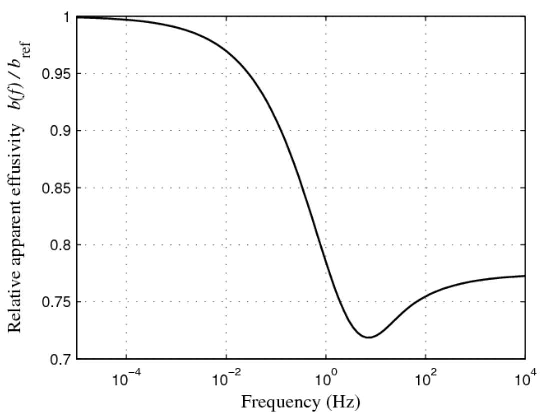


Profile $b(\xi)$ discretized into 507 slices ($\Delta b/b$<0.001)

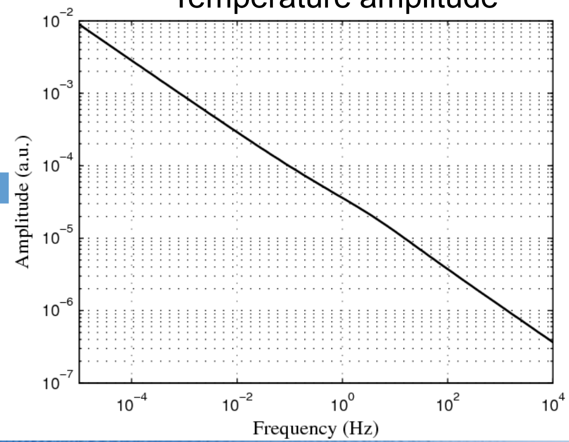
Temperature computation with classical quadrupoles

No "inversion crime"

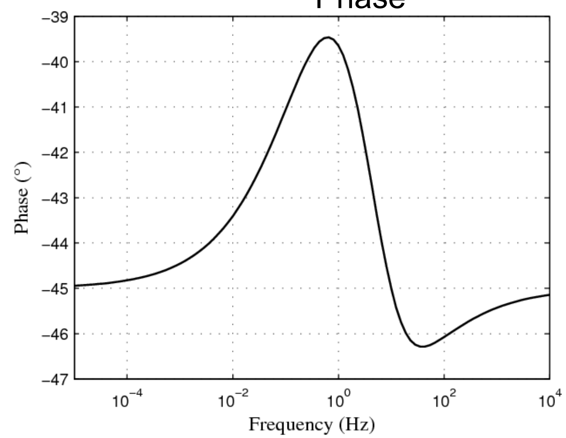
Apparent effusivity $b(f)$ (0-order inversion)



Temperature amplitude



Phase



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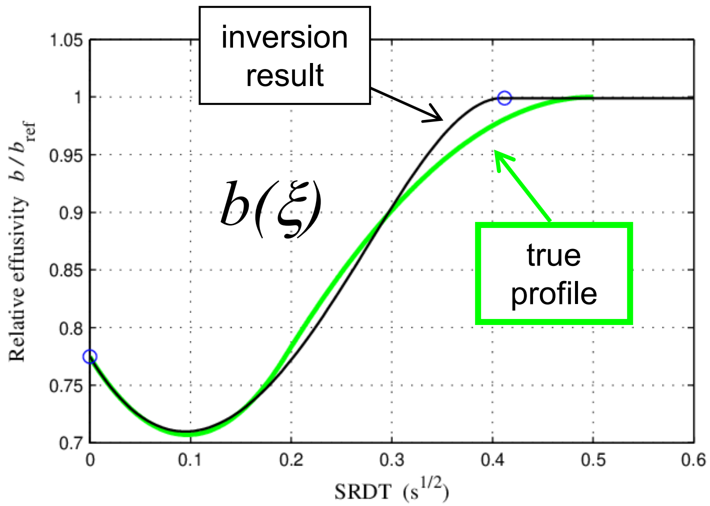
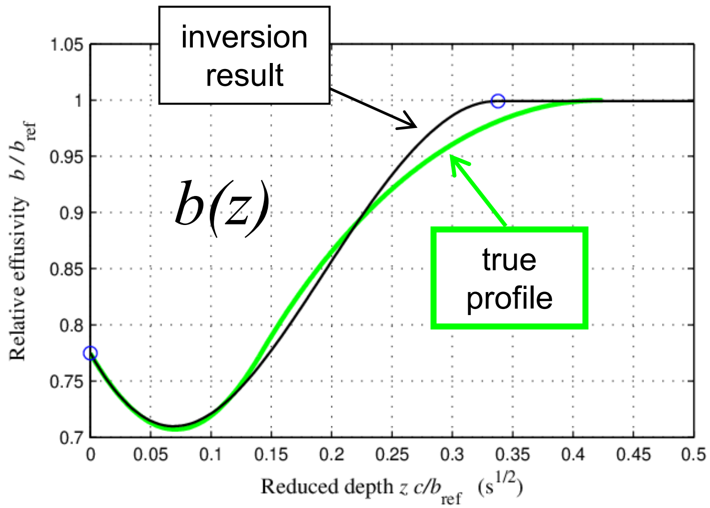
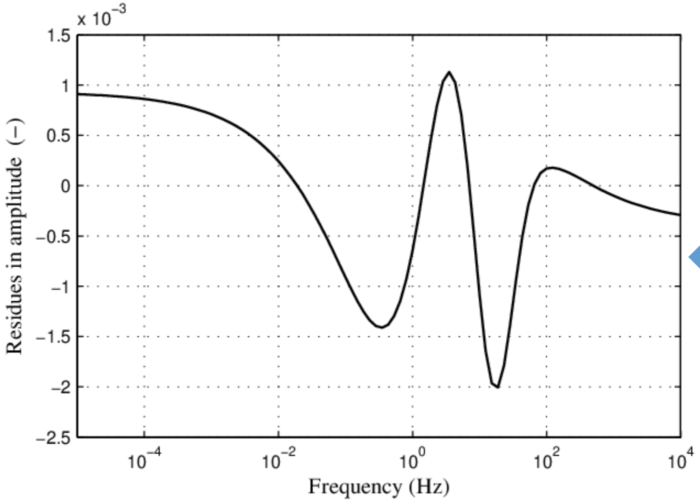
Inversion. Input data with no noise

Inversion attempt with *a priori* hypothesis on the unknown profile : **one *sech(ξ)* layer + uniform bulk**



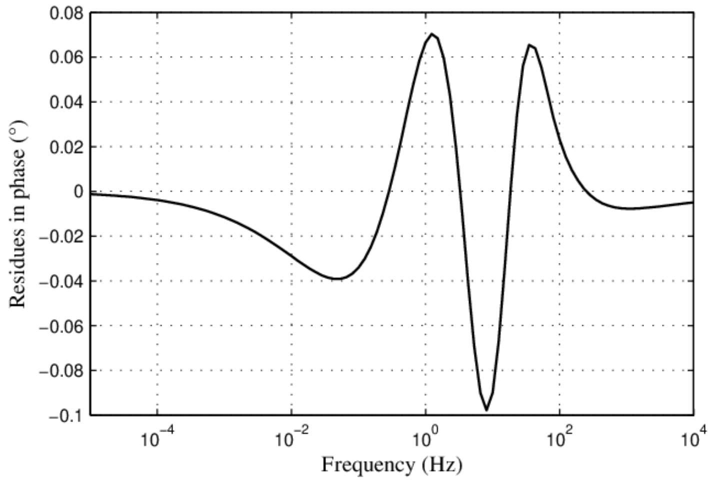




Temperature residues

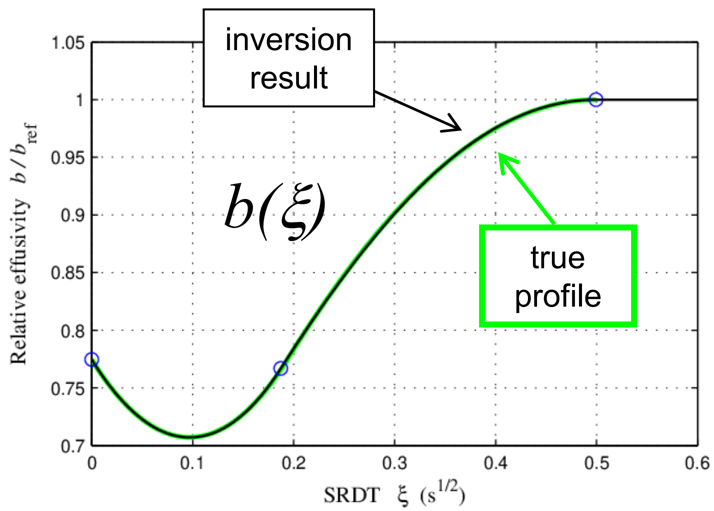
Amplitude

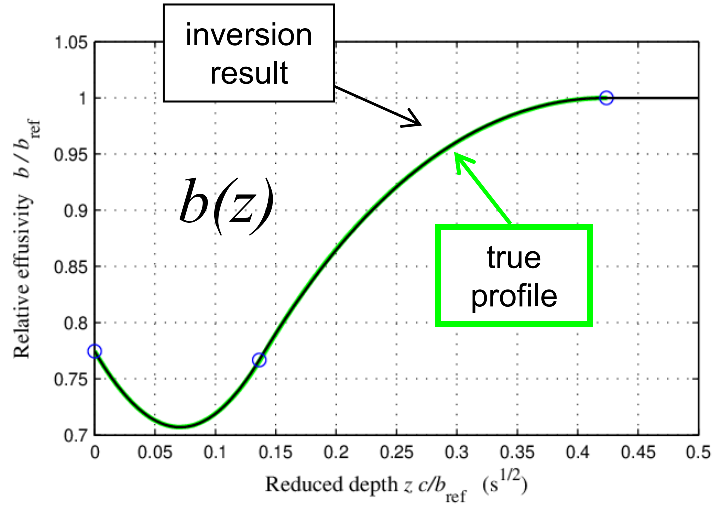
Phase

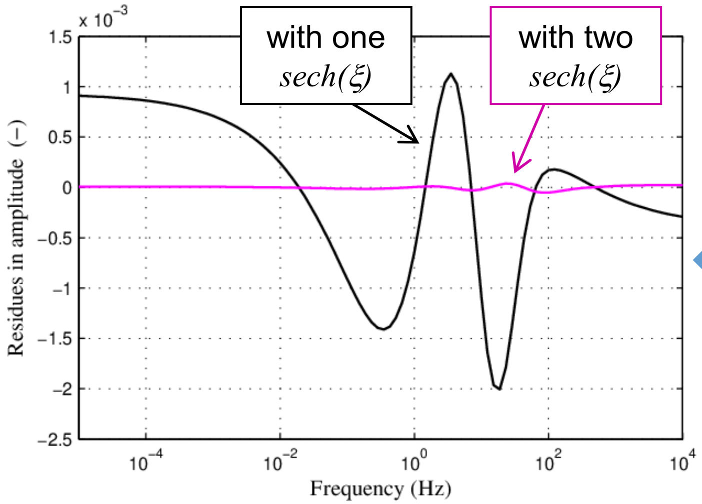


Inversion. Input data with no noise

Inversion attempt with *a priori* hypothesis on the unknown profile : **two *sech(ξ)* layers + uniform bulk**







Temperature residues

Amplitude

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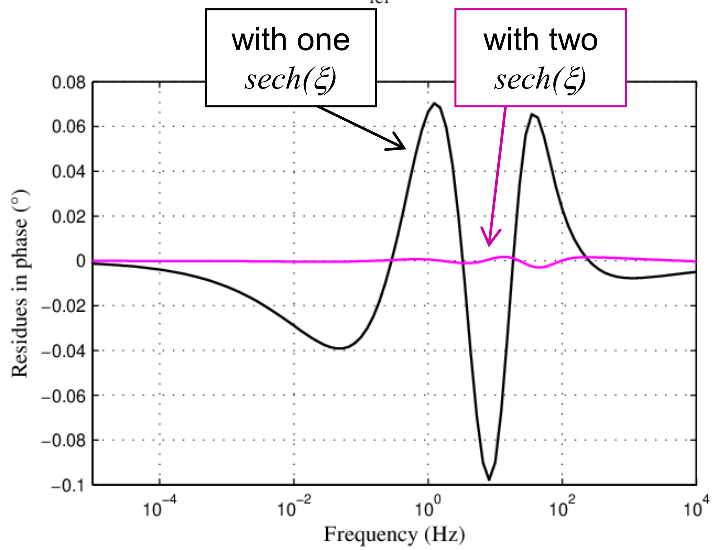

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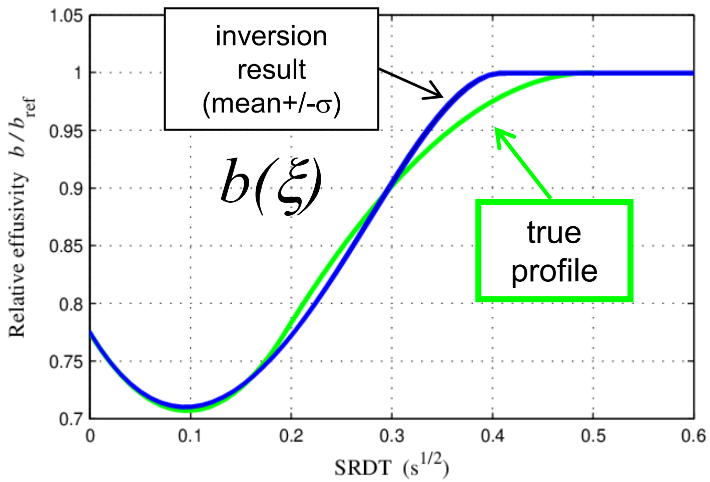
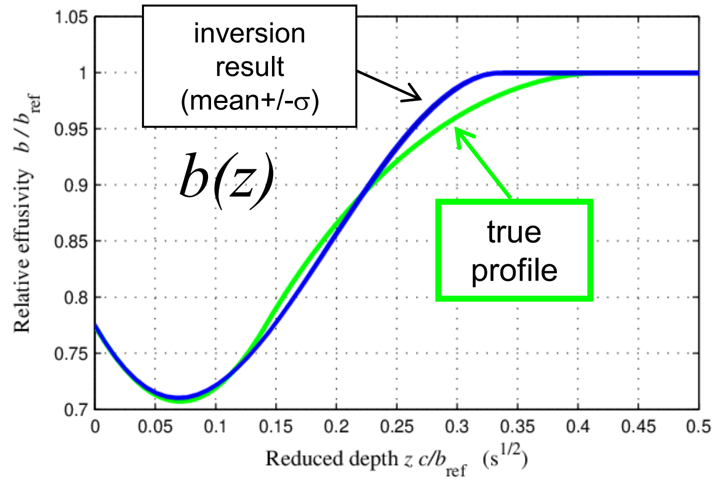
Inversion. Input data with noise (1% on amplitude, 0.1° on phase)

Inversion attempt with *a priori* hypothesis on the unknown profile : **one *sech(ξ)* layer + uniform bulk**

Statistics with 20 virtual experiments





Temperature residues

Amplitude

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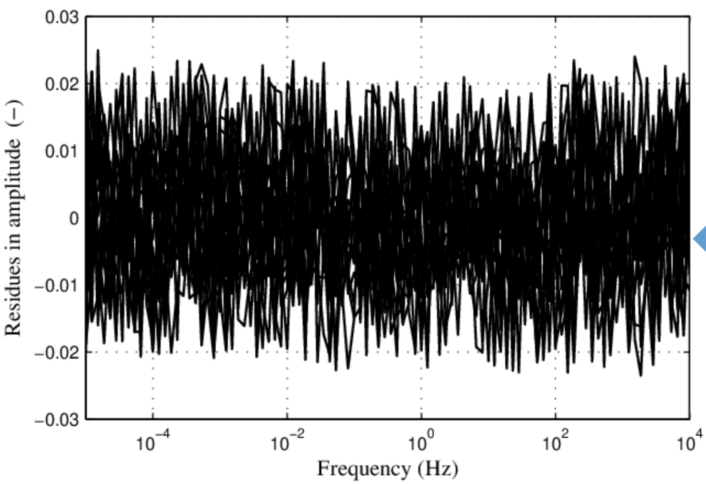

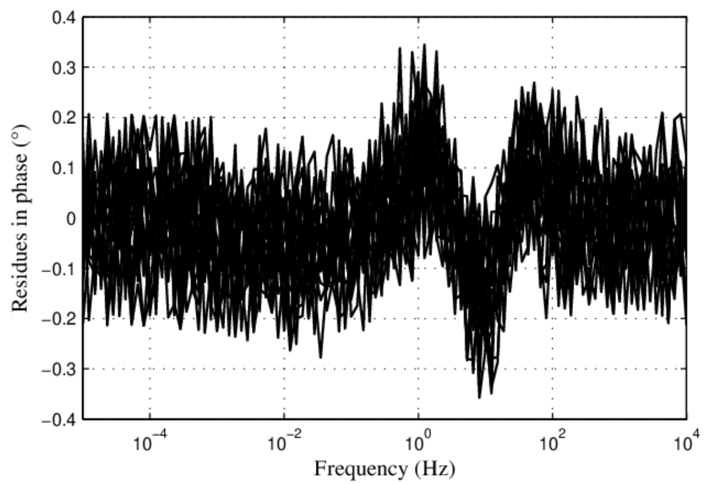

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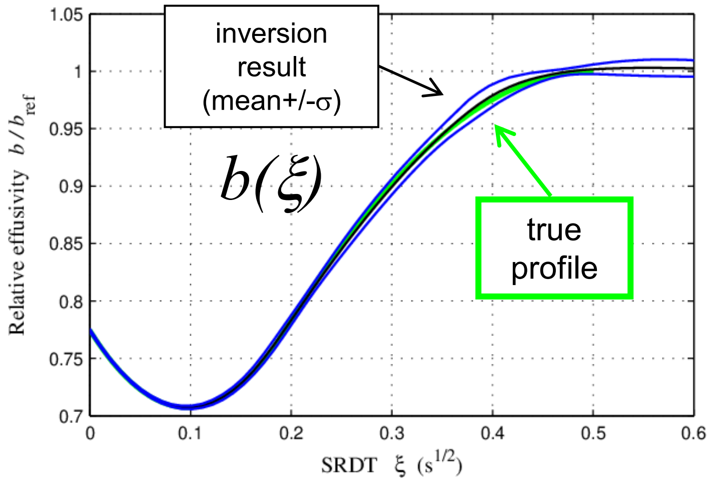
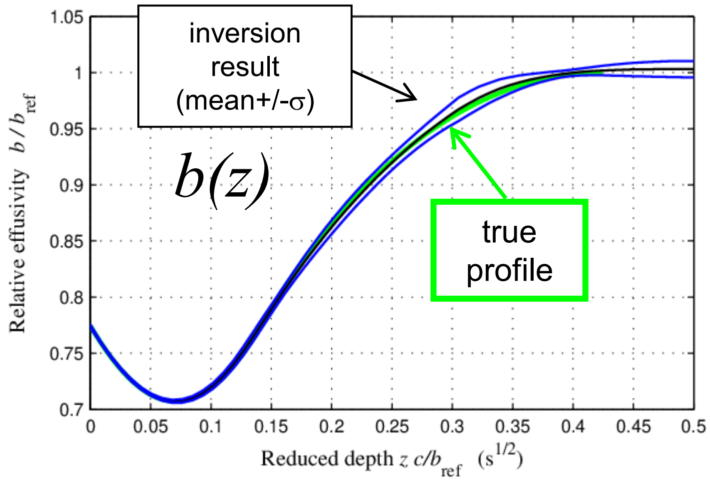
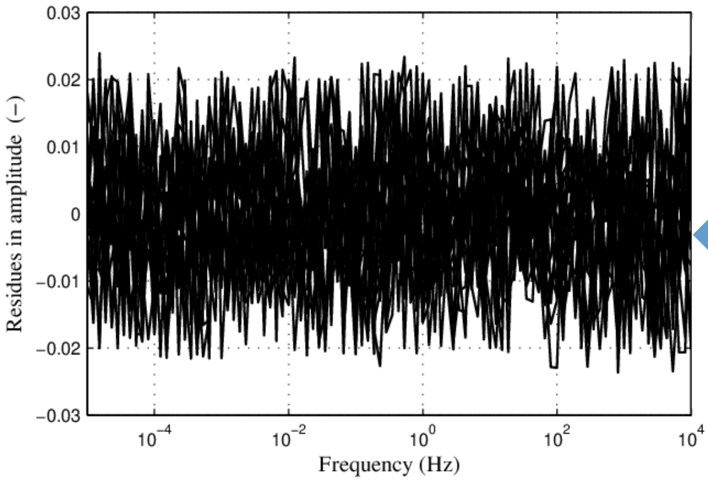


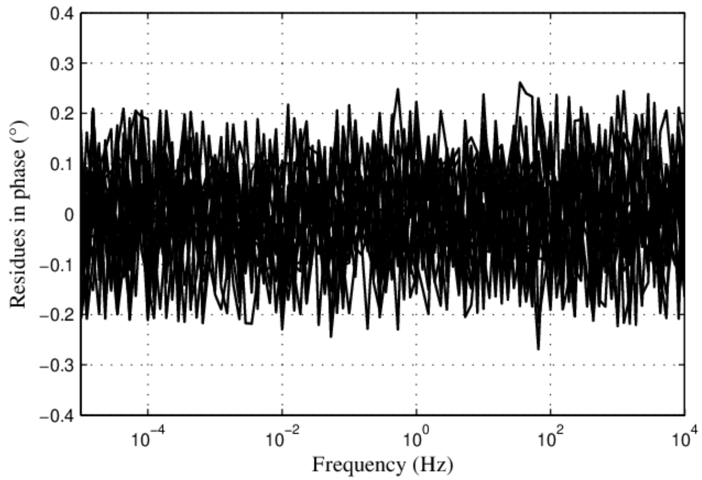




Temperature residues

Amplitude

Phase

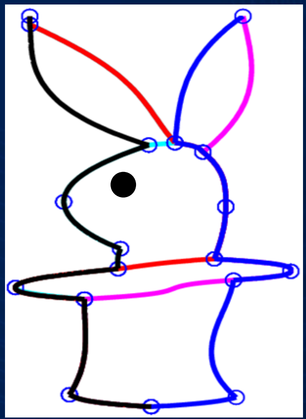


Thank you for your attention

Everything you always wanted to *know* about profiles (but were afraid to ask), is in:

$$\mathrm{sech}\left(\hat{\xi}\right)$$

Krapez, *Int. J. Heat Mass Tr.*, 99, 485 (2016)
Krapez, *J. Mod. Opt.*, 64, 1988-2016 (2017)
Krapez, *Int. J. Thermoph.*, 39:86 (2018)
Krapez, *J. Opt. Soc. Am.*, 35, 1039 (2018)



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