X ray Spectra reconstruction from analysis of attenuation data:

a Back Scattering Thomson Source application

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OVERVIEW

part I:

- formulation of our problem
- mathematics of regularization

part II:

- simulation of experiment and selection of algorithms
- experimental validation on filtered Bremsstrahlung spectra

part III:

- Thomson Sources Simulation

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why analyze attenuation data: Thomson Source example

10e9 photon per second
10 pulses 10 ps each

for conventional spectroscopy you need at most
1 photon per pulse without filtering the beam
and the machine working at full power

with a collimator of 50 um of diameter
the distance required is ~ 170 m

Our Problem:
spectrum estimation from attenuation measurements

attenuation measurements - monochromatic beam

$$\mathcal{N}(t) = \int_0^\infty \delta(E_0)\mathcal{N}_0 e^{-\mu(E)t} dE = \mathcal{N}_0 e^{-\mu(E_0)t}$$

polychromatic beam

$$\mathcal{T}(t) = \int_0^\infty \mathcal{X}(E) e^{-\mu(E)t} dE$$

suppose to know exactly $\mu(E)$ and t
and have an experimental measure of $\mathcal{T}(t)$

➡ is it possible to calculate $\mathcal{X}(E)$?

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Our Problem:
discrete formulation

polychromatic beam

$$\mathcal{T}(t) = \int_0^\infty \mathcal{X}(E) e^{-\mu(E)t} dE$$

compact linear operator: its inverse is not continuous

discretization

$i = 1 \ldots m$ measurements

$j = 1 \ldots n$ energy bins

$$T = AX$$

$A \in \mathbb{R}^{mxn}, T \in \mathbb{R}^m$ e $X \in \mathbb{R}^n$

it turns out in a linear system which is highly ill-conditioned

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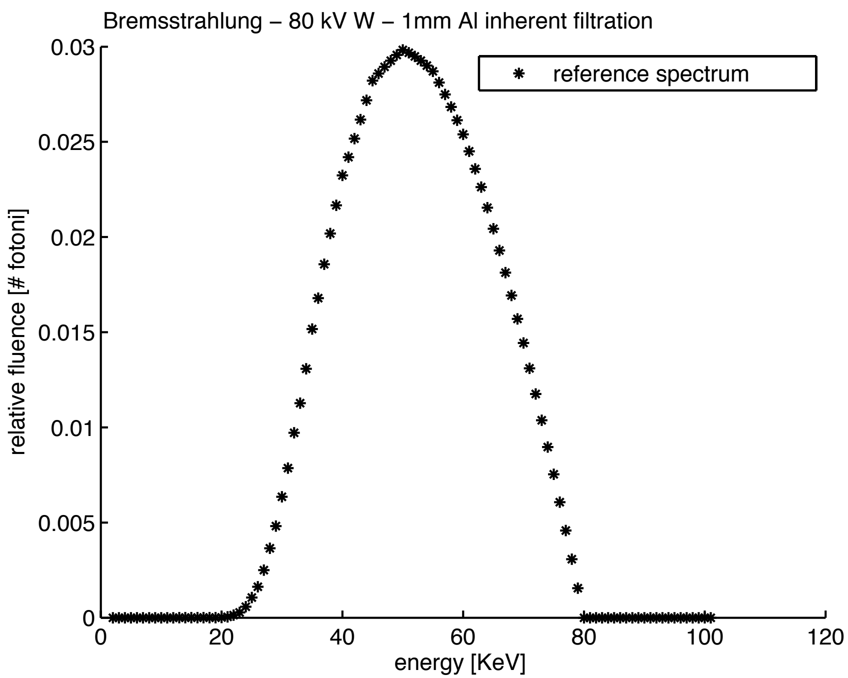
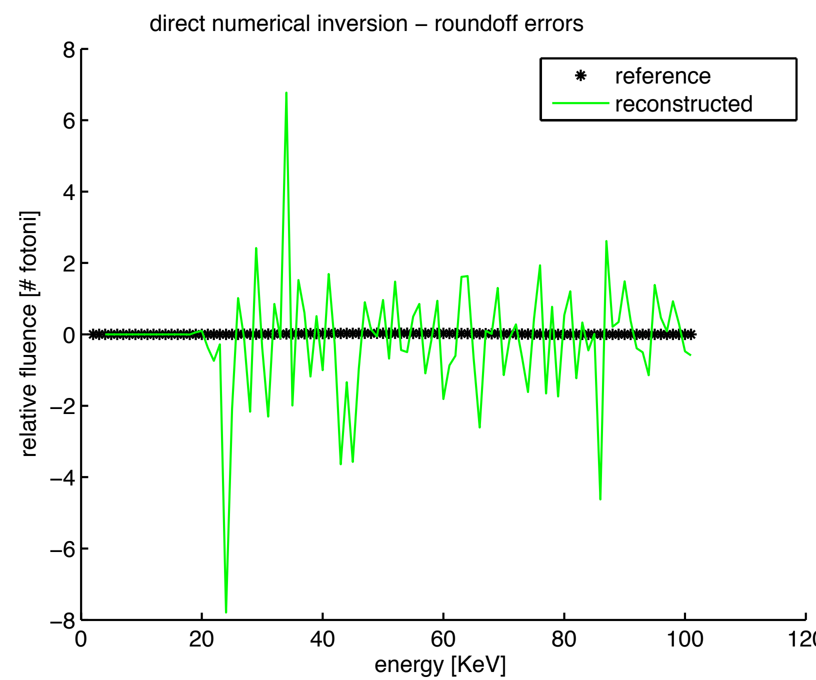
an example: direct reconstruction in attenuation data is present only round-off noise



$$cond(A) = 1.4 \times 10^{20}$$



the propagation of noise is strong enough to completely destroy any information about the original spectrum

$$X = A^{-1}T$$

ill-conditioning:
what does it mean?

- the system shows instability due to extreme sensitivity to the noise
- there is a serious dump of the information of the initial physical state during the evolution of the system

ill-conditioning:
what can we do

- the system shows instability due to extreme sensitivity to the noise

- there is a serious dump of the information of the initial physical state during the evolution of the system

- ill-conditioning does not mean that NO information can be extracted but simply that STANDARD METHODS in numerical linear algebra cannot be applied in a straightforward way

- we need some A PRIORI or EXTRA information about the solution we are looking for in order to compute a useful APPROXIMATION to the exact, unknown solution

Our Problem:
abstract representation

let us formulate our problem in a slightly more abstract way, consider a compact linear operator

$\mathcal{K}$ which acts between two Hilbert Spaces $\mathcal{G}$ and $\mathcal{F}$

$$\mathcal{K} : \mathcal{F} \to \mathcal{G}$$

now the problem can be represented as

$$g = \mathcal{K} f$$

where $\mathcal{K}$ is the model

$g \in \mathcal{G}$ the measurements

$f \in \mathcal{F}$ the uknwown solution

noise in the measurements

moreover, we know the attenuation curve only through measurements

$$g_{exp} = g + \delta$$

with δ the experimental error

even imposing $\dfrac{||\delta||}{||g||}$ to be small

the solution obtained as

$$f_{exp} = \mathcal{K}^{-1} g_{exp}$$

will be compromised by the noise propagation

$$\frac{||\Delta f||}{||f||} \leq cond(\mathcal{K}) \frac{||\Delta g||}{||g||}$$

Regularization Operator:
definition

$$\mathcal{K} : \mathcal{F} \to \mathcal{G}$$
$$\alpha(\delta, g_{exp}) \in [0, \infty)$$

given a compact operator and a real, non negative parameter

consider the continuous operator

$$\mathcal{R}_\alpha : \mathcal{G} \to \mathcal{F}$$

the family of operators $\{\mathcal{R}_\alpha\}$

is called a regularized operator for $\mathcal{K}^\dagger : \mathcal{G} \to \mathcal{F}$

and has the following properties

$$\lim_{\delta \to 0} \sup\{||\mathcal{R}_\alpha g_{exp} - \mathcal{K}^\dagger g||\} = 0$$

$$\lim_{\delta \to 0} \sup\{\alpha(\delta, g_{epx})\} = 0$$

Tikhonov Regularization: a penalty method

the basic idea of Tikhonov-type regularization is to minimize the residual and, at the same time, to impose a bound on the size of the computed solution

$$X_\lambda = argmin_X \left\{ ||T_{exp} - AX||_2^2 + \lambda^2 ||X||_2^2 \right\}$$

$$\lambda \in [0, \infty)$$

there are two equivalent formulation that can be useful to compute the approximation to the solution

$$\min \left\| \begin{pmatrix} A \\ \lambda \end{pmatrix} X - \begin{pmatrix} T_{exp} \\ 0 \end{pmatrix} \right\|$$ and $$(A^t A + \lambda^2 I) X = A^t T_{exp}.$$

TSVD Truncated Singular Value Decomposition
a projection method

the starting point is the Singular Value Decomposition of the linear system which is defined as:

$$A = U\Sigma V^t \qquad A \in \mathbb{R}^{m\times n} \text{ with } m \leq n$$

$$\Sigma = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ 0 & \cdots & 0 \\ \vdots & \ddots & 0 \\ 0 & \cdots & 0 \end{bmatrix}$$

$$U \in \mathbb{R}^{m\times m}, \Sigma \in \mathbb{R}^{m\times n}, \text{ and } V \in \mathbb{R}^{n\times n}$$

so that we can express the approximation to the solution in this way:

$$A^\dagger T_{exp} = \sum_{i=1}^{r} \frac{u_i^t T_{exp}}{\sigma i} v_i = \sum_{i=1}^{r} \left(\frac{u_i^t T}{\sigma i} v_i + \frac{u_i^t e}{\sigma_i} \right)$$

TSVD Truncated Singular Value Decomposition a projection method

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“exact” term contribution
no divergence problem

noise contribution: is likely to diverge when i becomes big; the singular values decreases while noise components does not

the idea is to truncate the sum when the singular values become too small compared to the level of noise, the solution is simply:

$$X_k = \sum_{i=1}^{k} \frac{u_i^t T_{exp}}{\sigma_i} v_i$$

it’s just the projection over the first k singular vectors

Maximum Likelihood method:
statistical iterative algorithm

- iterative algorithm: request an input spectrum and a stopping rule
- each approximation X^k to the spectrum is guaranteed to be non-negative
- the mean intensity of AX^k is conserved each iteration
- simple implementation

$$X_n^{k+1} = X_n^k f_n$$

$$f_n = \frac{\sum_m {A^t}_{nm} \frac{T_m}{\sum_{n'} A_{mn'} X_{n'}^k}}{\sum_m {A^t}_{nm}}$$

Maximum Likelihood method: the case of Poisson Noise

- iterative algorithm: request an input spectrum and a stopping rule
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in the case of Poisson Noise
the Maximum Likelihood Method
looks like this
[Richardson-Lucy]
or
[Expectation Maximization]

Expectation Maximization algorithm:
a priori spectrum and stopping rule

input distribution

FLAT: we are not imposing any constraint to the spectral distribution

SHAPED: for example we know that there are no photons above a certain energy

discrepancy principle

$$||T_{meas} - AX^k||_2 = \delta$$

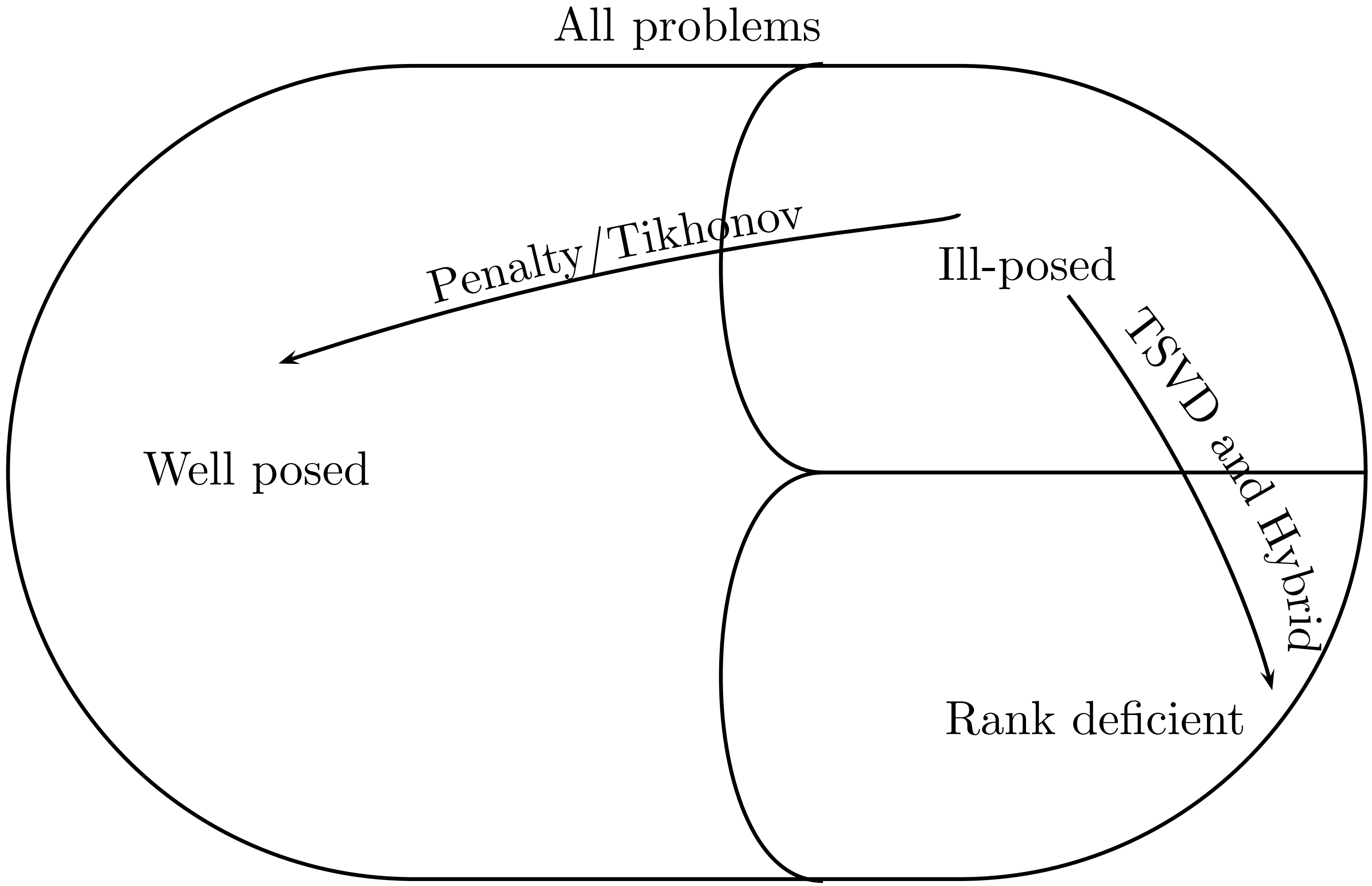
we can't expect to have a better approximation to the attenuation curve from computed spectra with respect to the direct measurements

$$T_{meas} = T_{exact} + e$$

$$d = ||e||_2$$

when $\delta(k) \leq d$ we stop the iterations

Regularization in a picture



we need some EXTRA knowledge, for example form the physics that governs the experiment, to choose some constrains or to project over a good subspace

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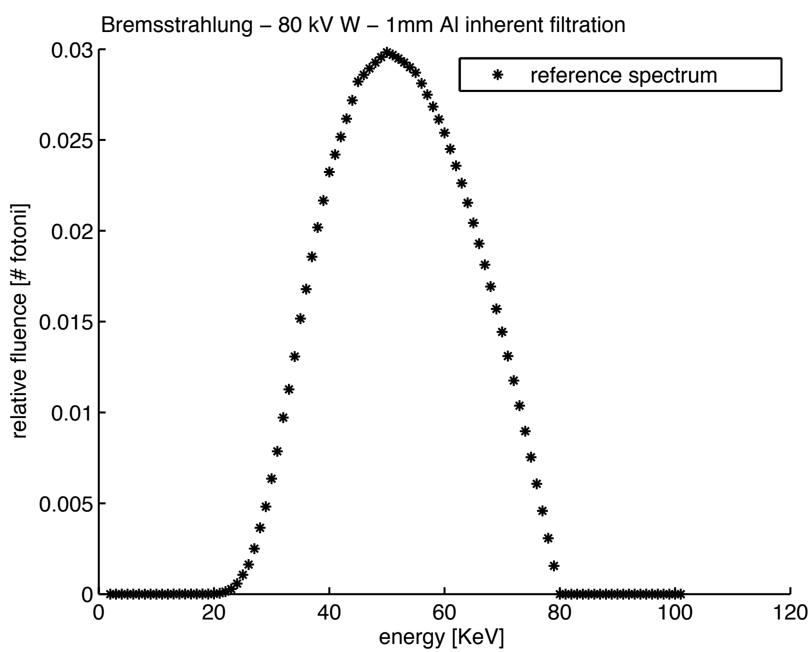
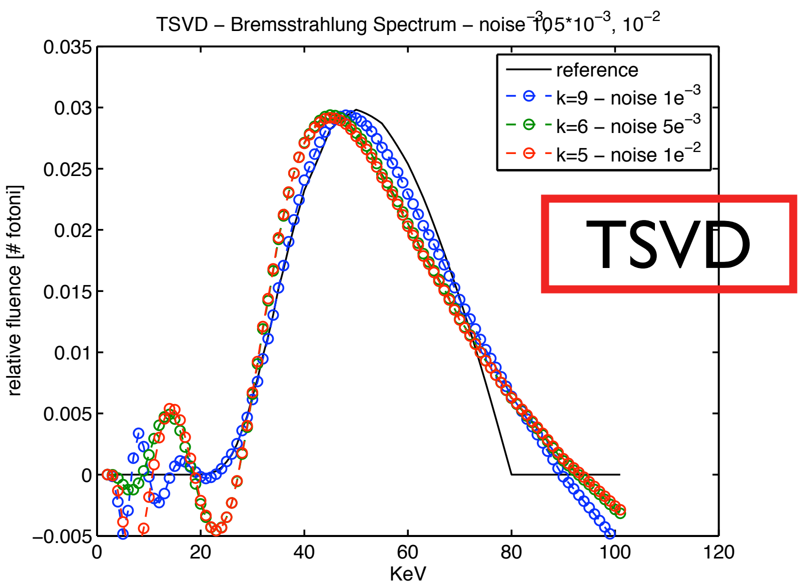
Simulations & Figure Of Merit

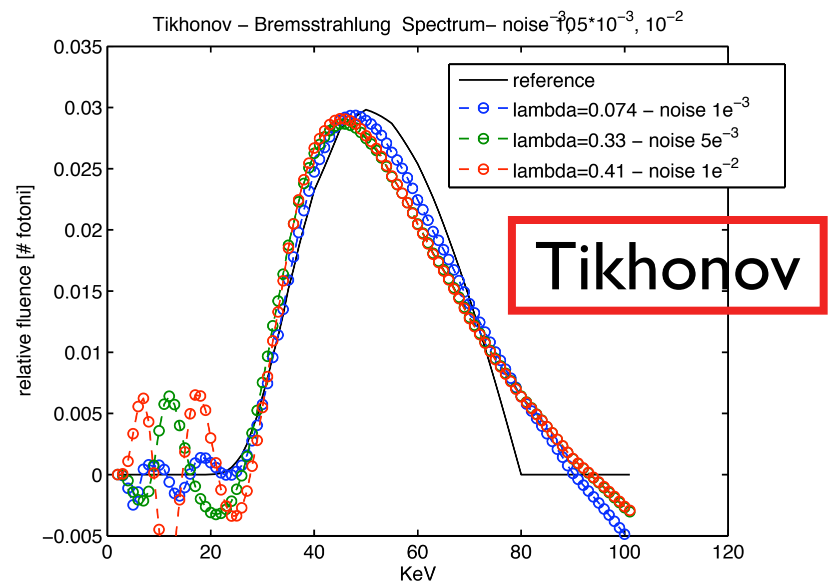
SIMULATED EXPERIMENT:
80 kV - W anode with 1mm Al inherent filtration
the attenuation curve is computed in Al
the curve is perturbed with three different level of noise
comparison of different methods for spectrum estimation

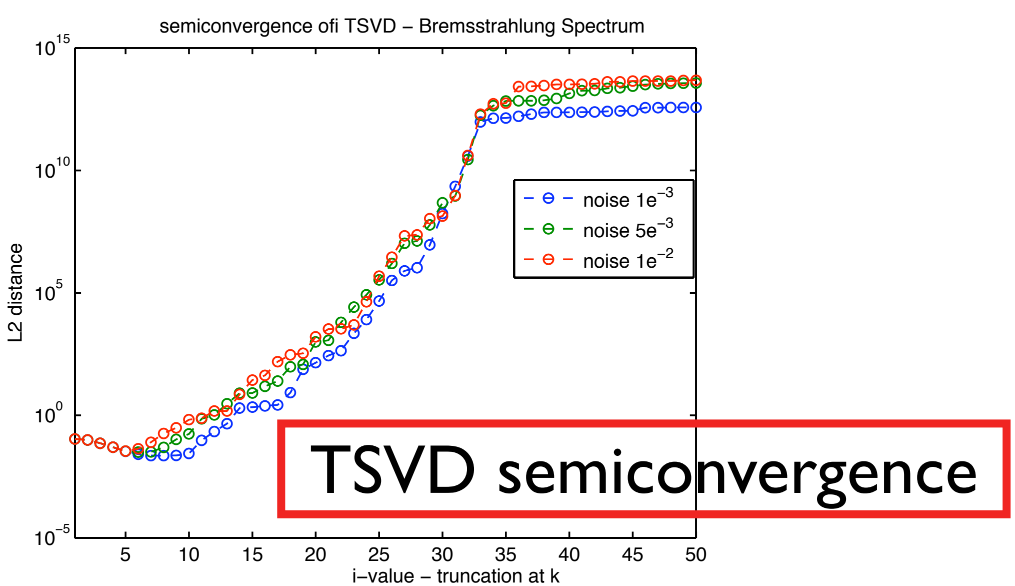


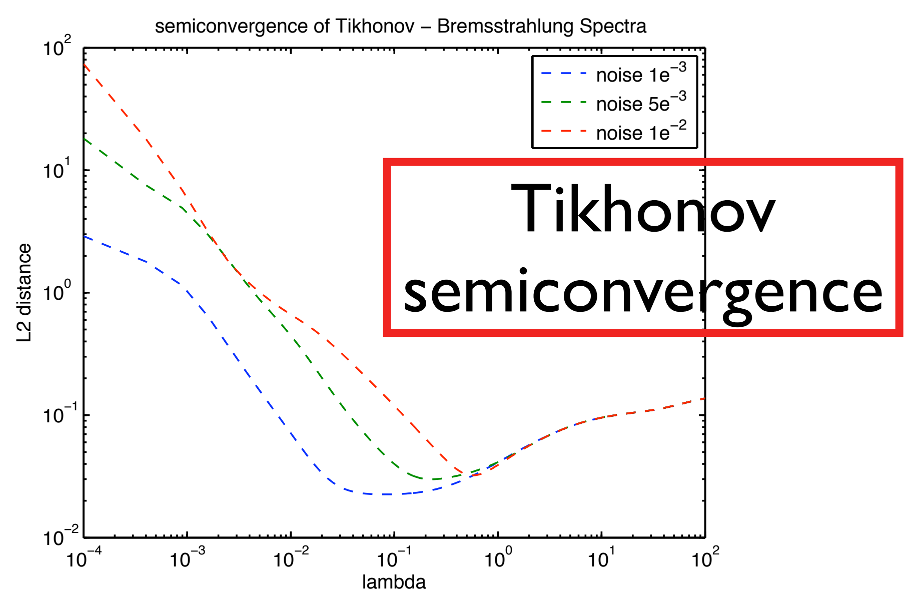
as we are interested in the SHAPE of the spectrum we choose an L2 distance criterion to study convergence properties of different algorithms

Simulations & FOM: TSVD and Tikhonov

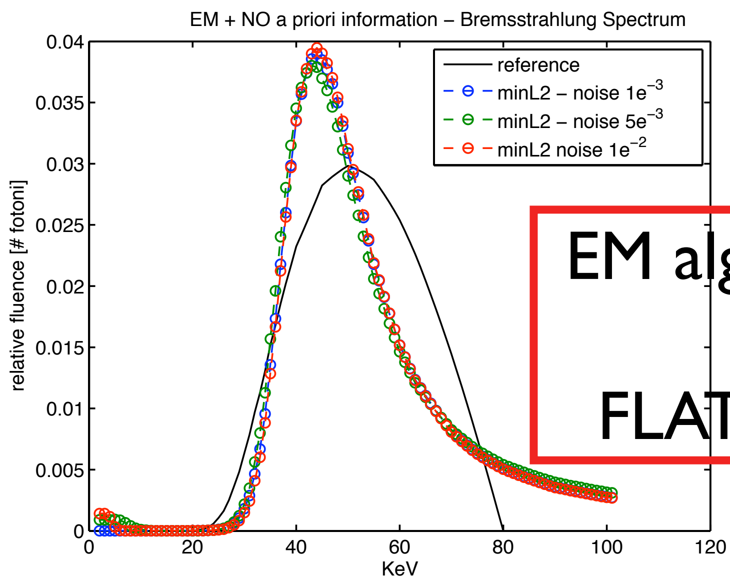




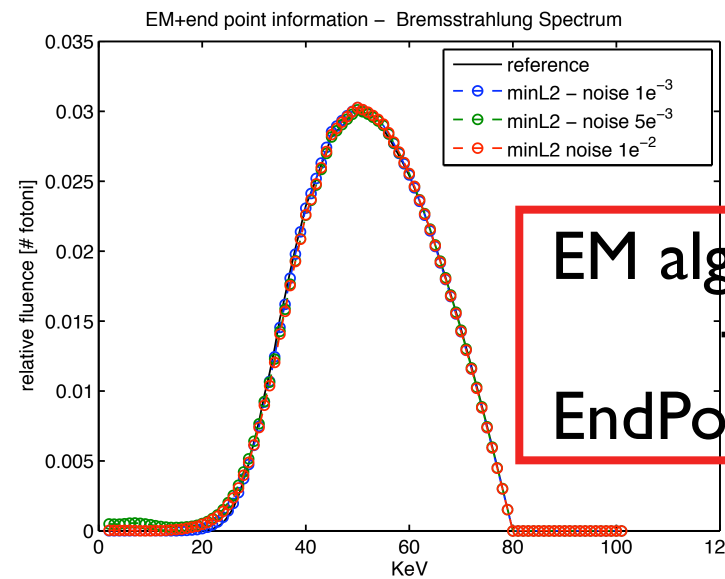




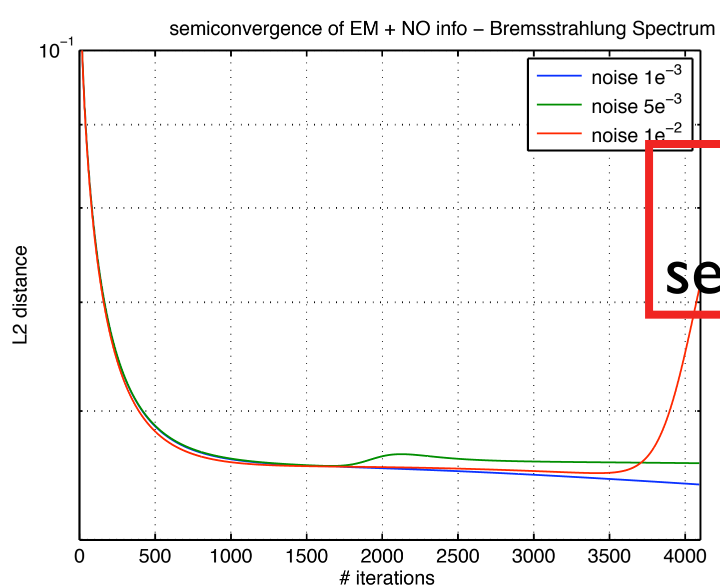
Simulations & FOM:
Expectation Maxmization



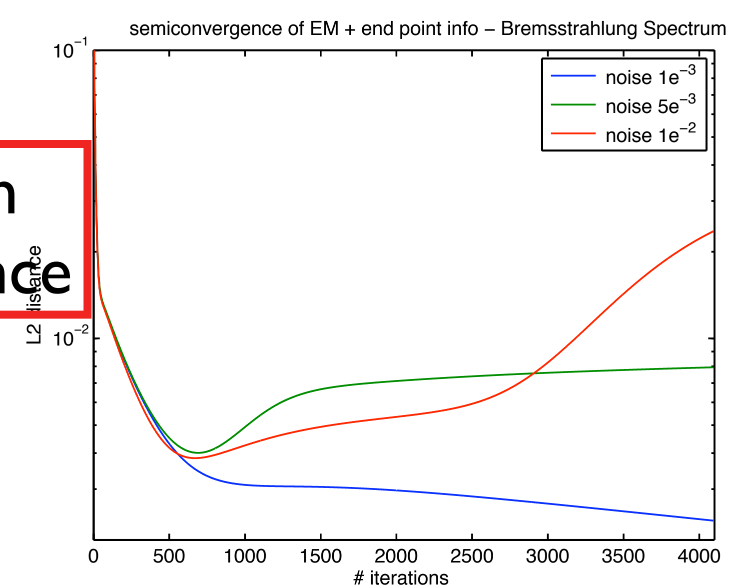
EM algorithm
+
FLAT prior



EM algorithm
+
EndPoint info

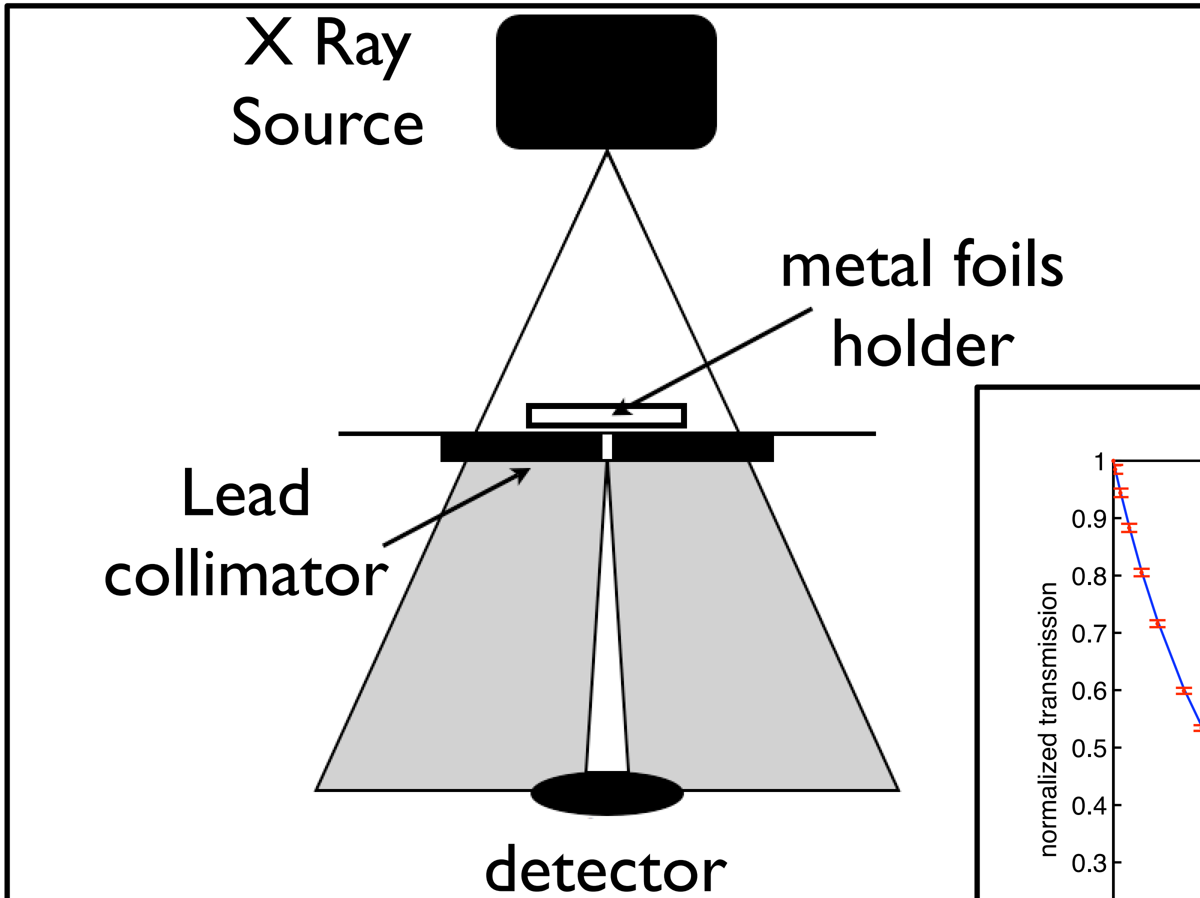


EM algorithm
semiconvergence

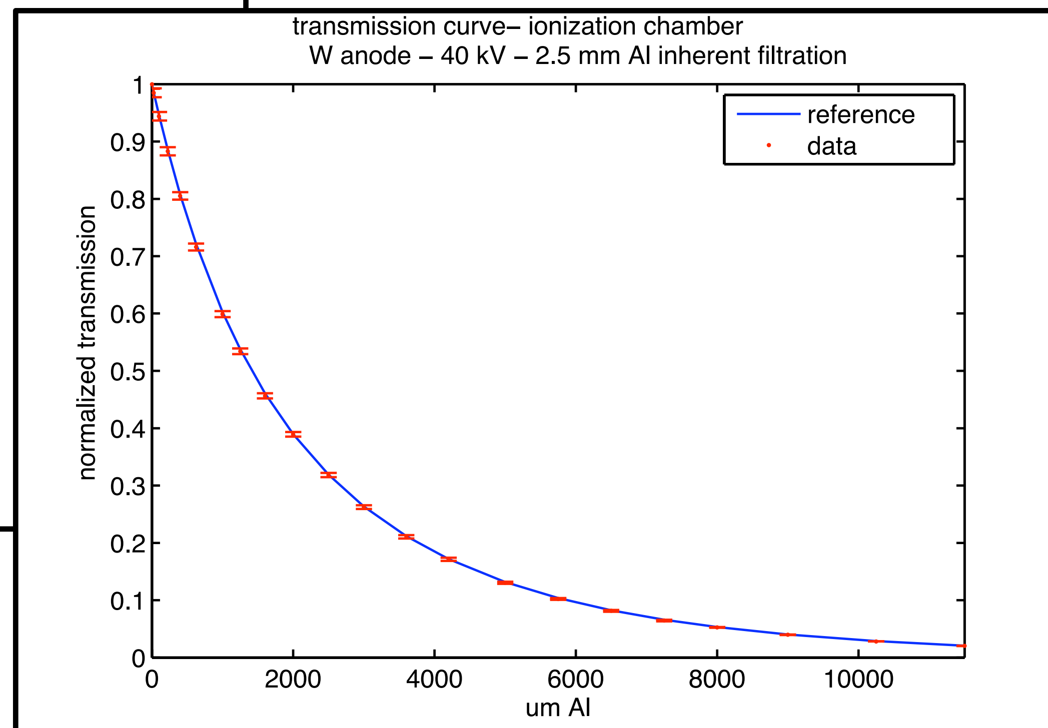


Experimental Validation: set up

experimental set-up

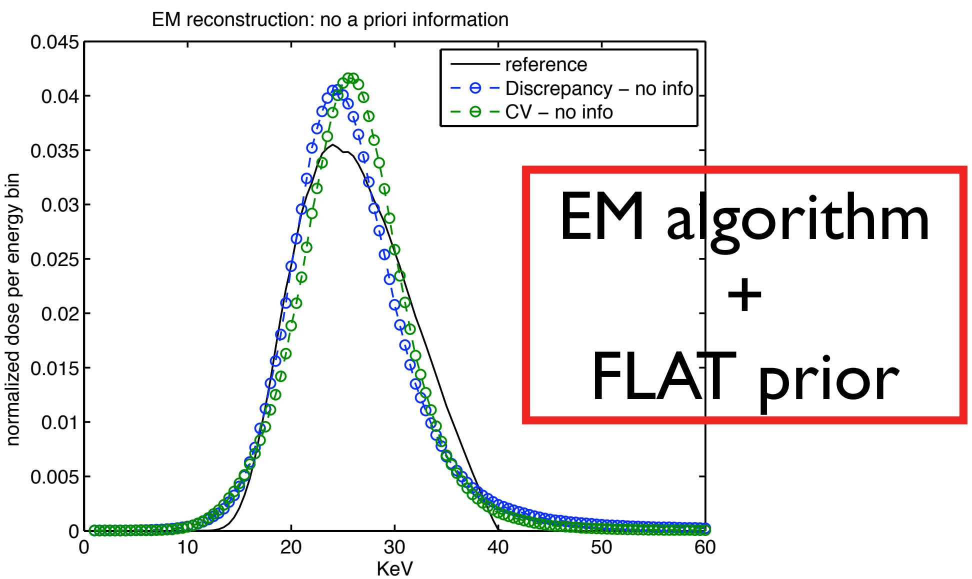


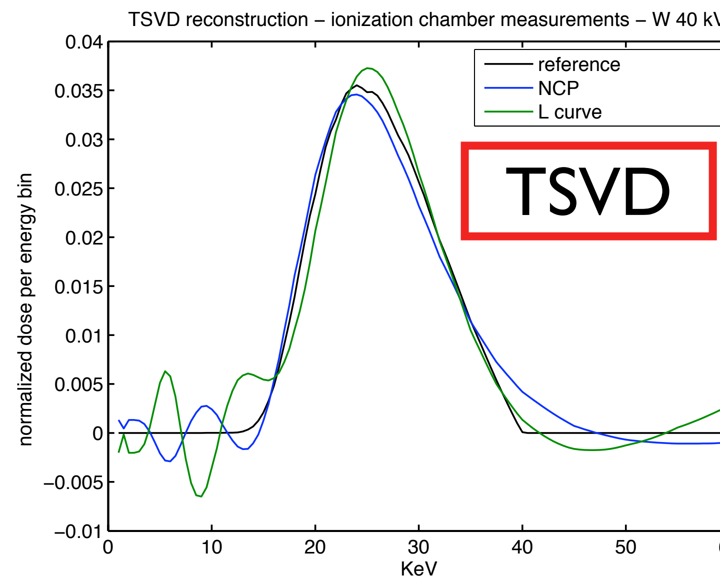
transmission curve
22 measurements Al

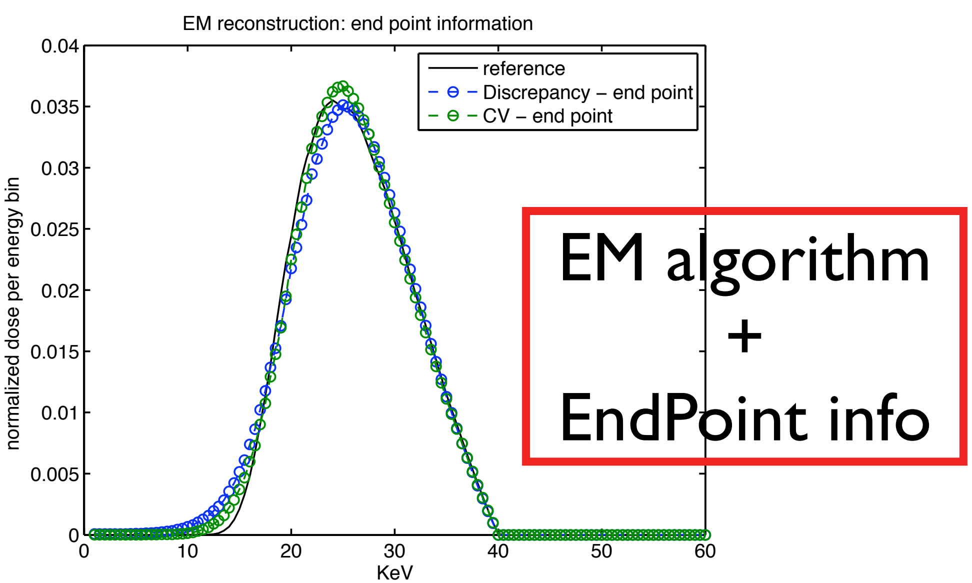


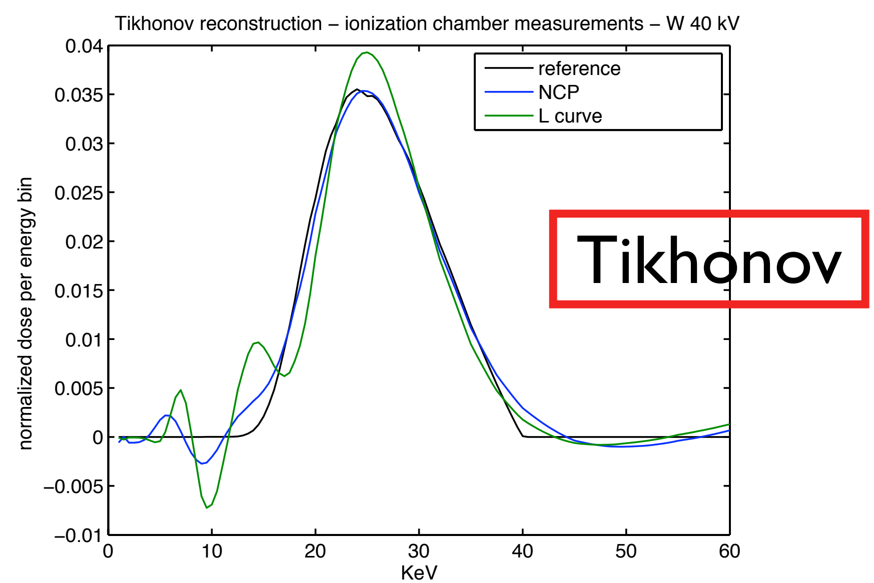
- background radiation
- scattering

Experimental Validation:
40 kV - W anode - 2.5 mm Al inherent filtration









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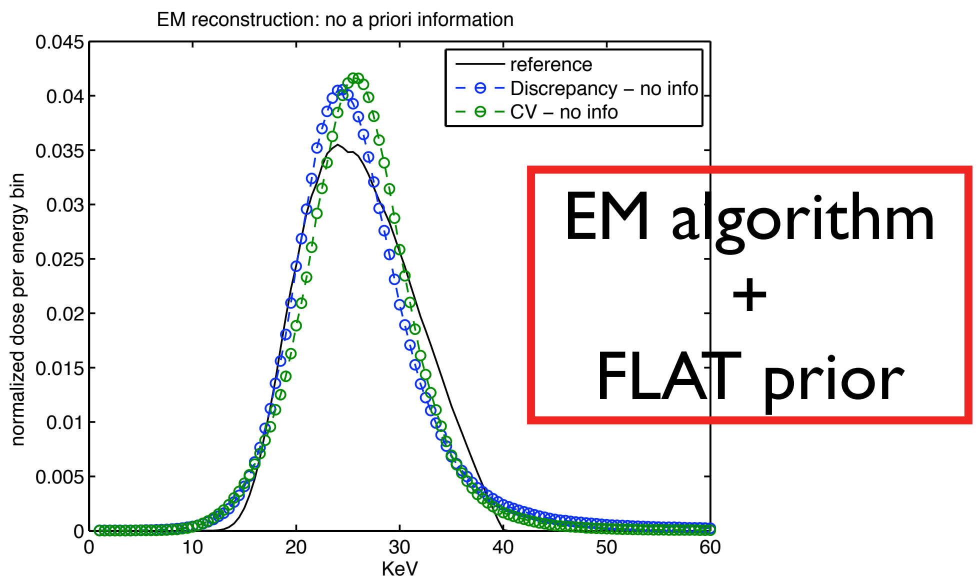
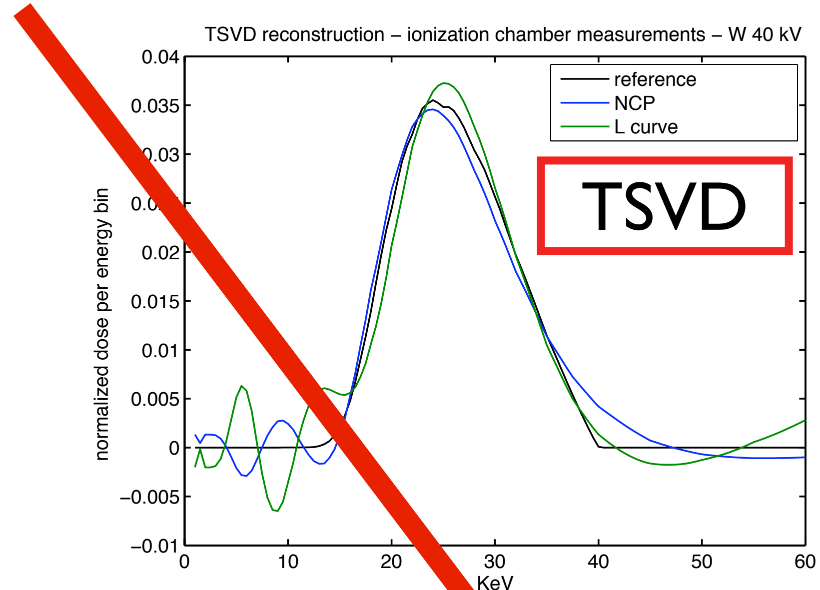
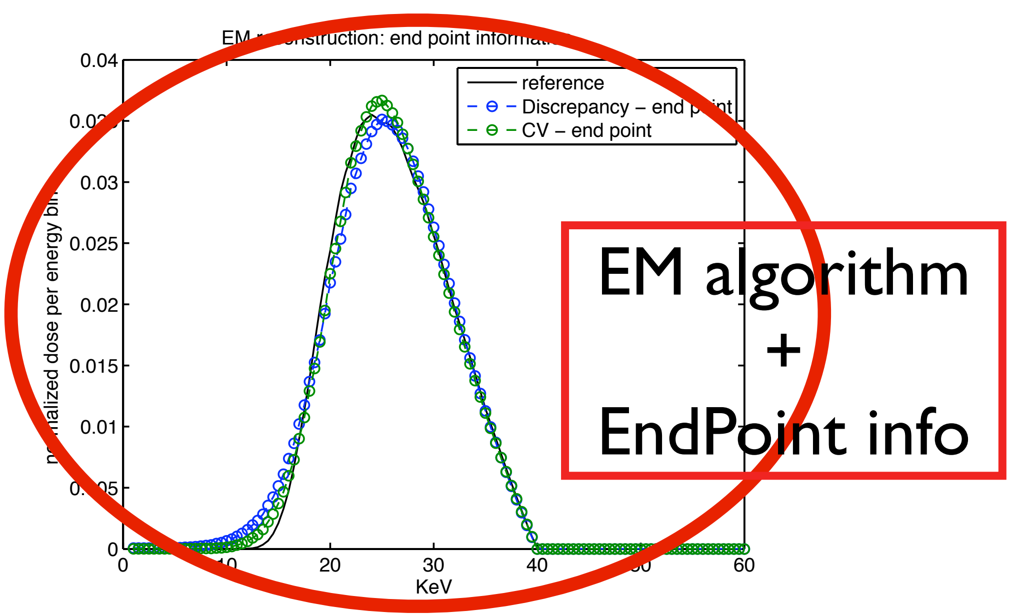
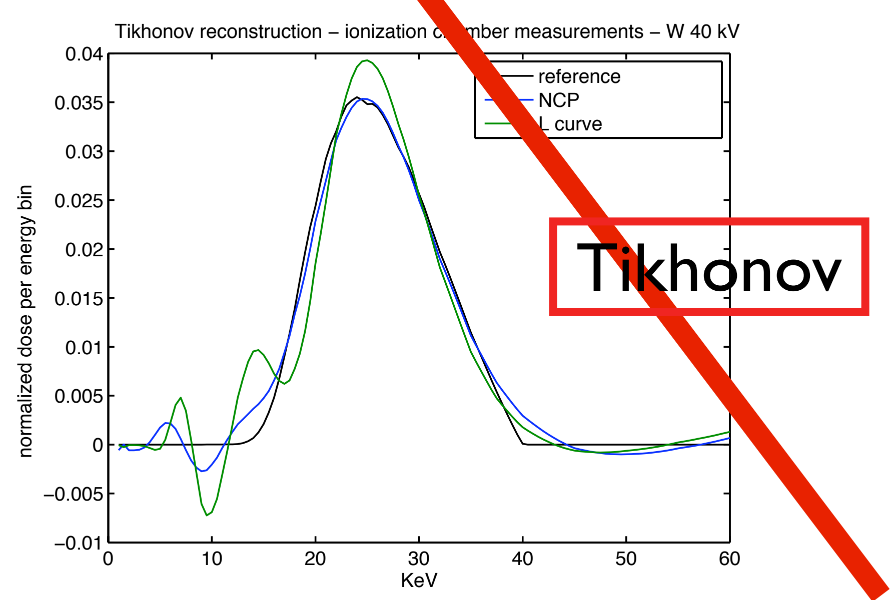
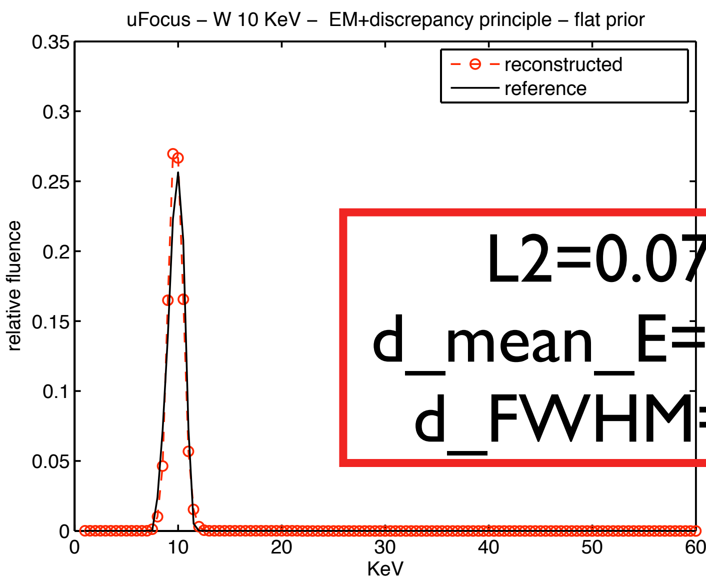




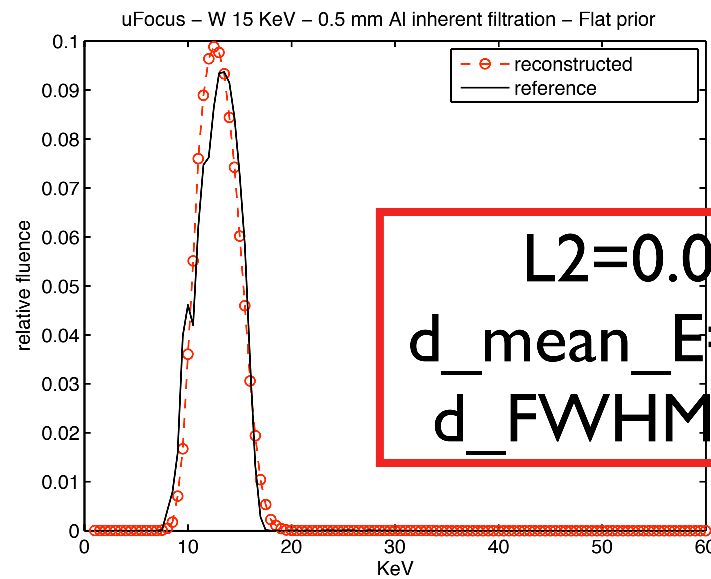




Experimental Validation:
10,15,20 kV - W anode - 0.5 mm Al filtration



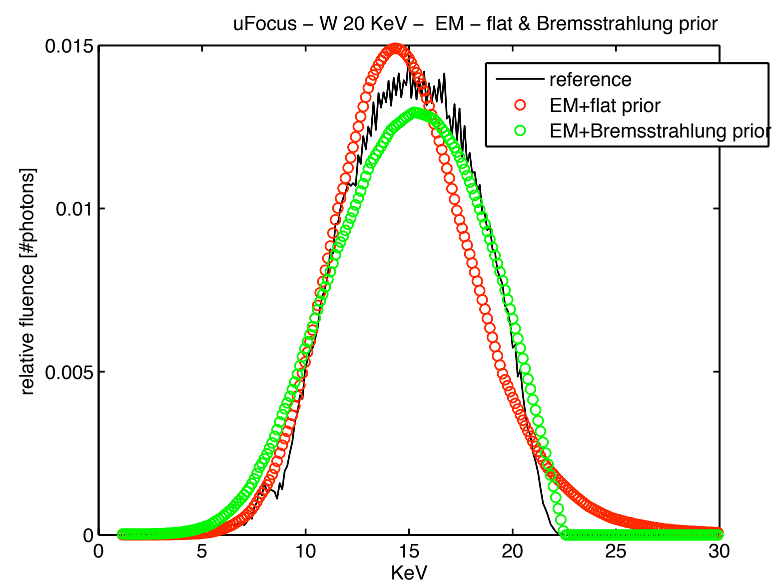
L2=0.073
d_mean_E=0.001
d_FWHM=0.1



L2=0.054
d_mean_E=0.015
d_FWHM=0.03

Relative Errors

L2 distance flat prior = 0.0175
d_mean flat prior = 0.006
d_FWHM flat prior = 0.09
L2 distance end-point info = 0.0125
d_mean end-point info = 0.005
d_FWHM end-point info = 0.02



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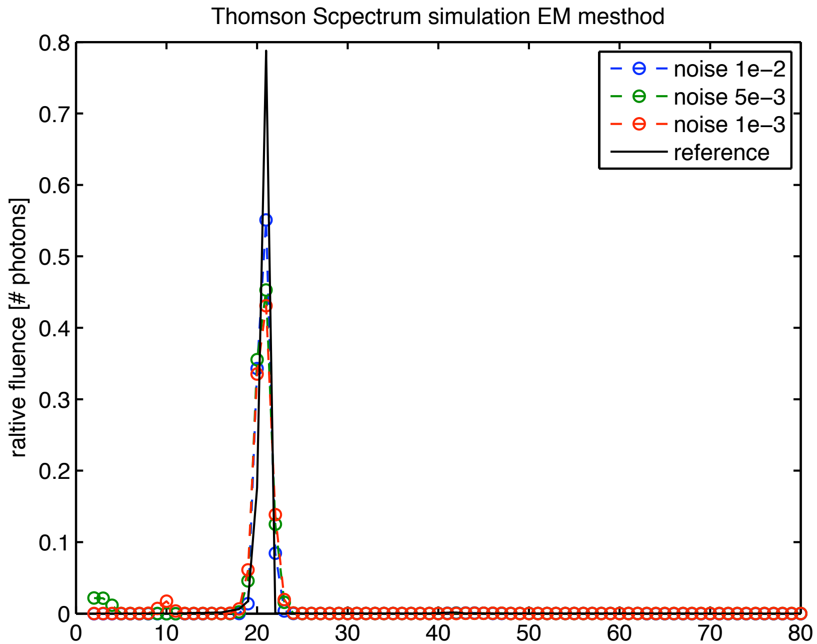
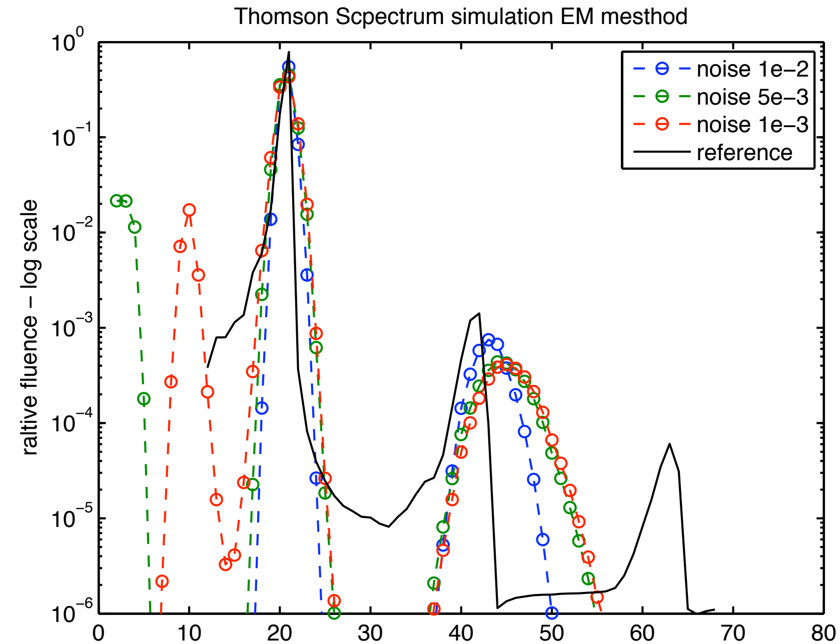
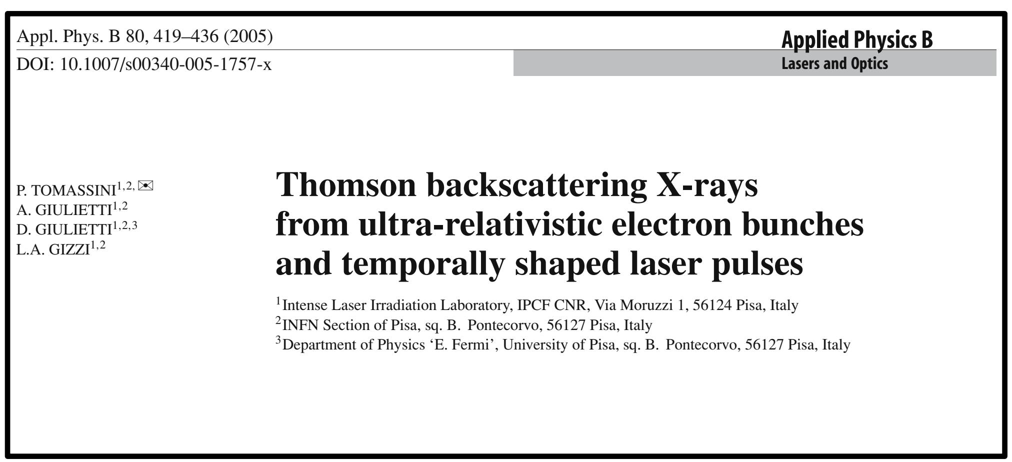
Thomson Source Simulations: Expectation Maximization Algorithm







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Applied Physics B

Lasers and Optics

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Thomson backscattering X-rays from ultra-relativistic electron bunches and temporally shaped laser pulses

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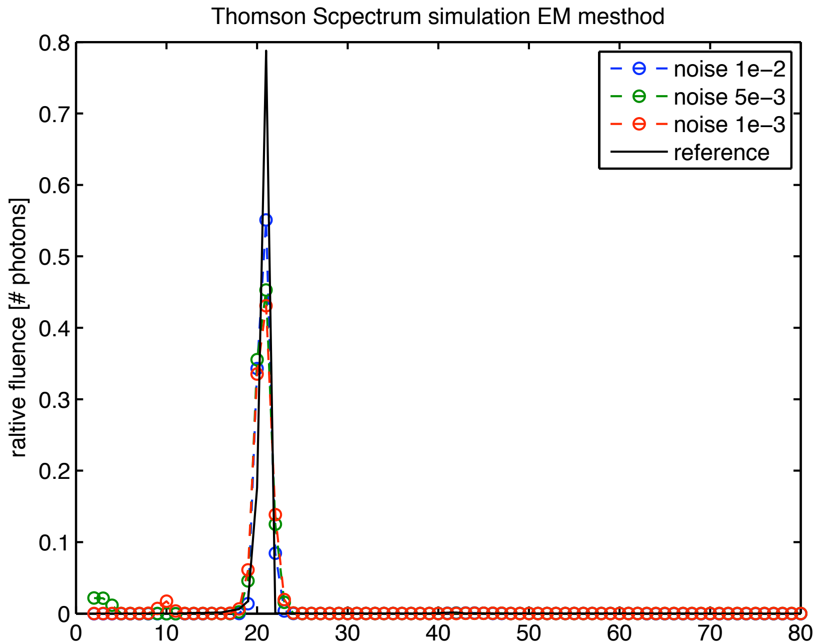
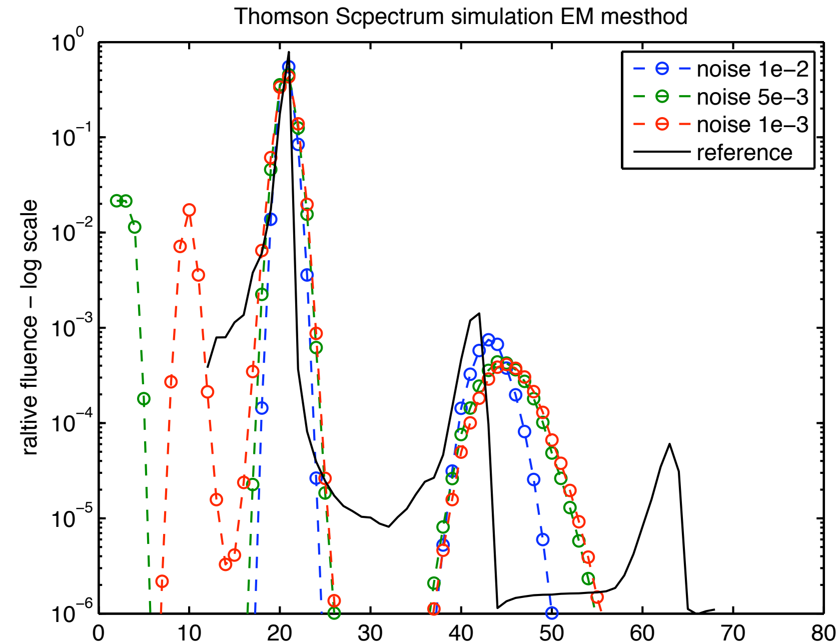
Thomson Source Simulations:
Expectation Maximization Algorithm

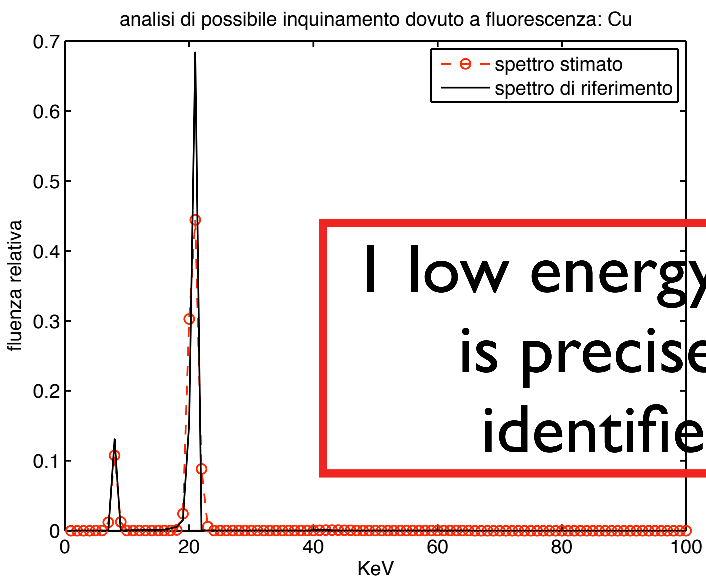




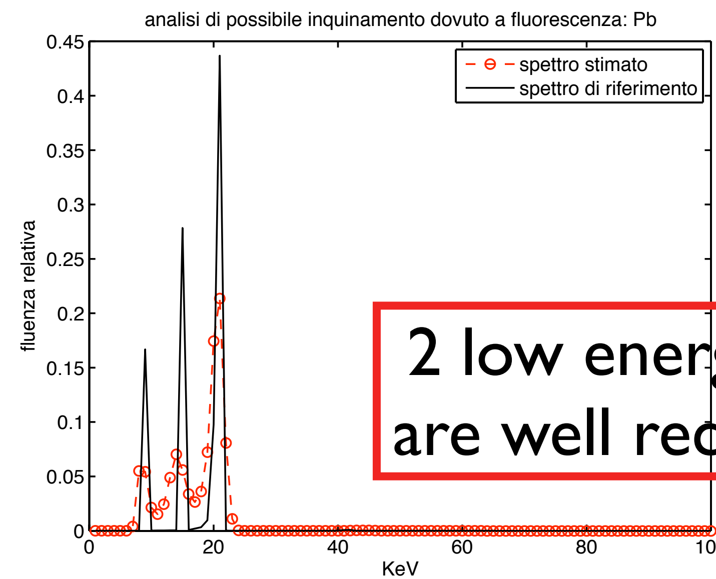
Relative Errors

Mean Energy	1st Harmonic Peak	Total Area
noise 1e-2 = 0.001	noise 1e-2 = 0.1	noise 1e-2 = 0.008
noise 5e-3 = 0.006	noise 5e-3 = 0.4	noise 5e-3 = 0.01
noise 1e-4 = 0.007	noise 1e-4 = 0.3	noise 1e-4 = 0.02
excellent	poor	good

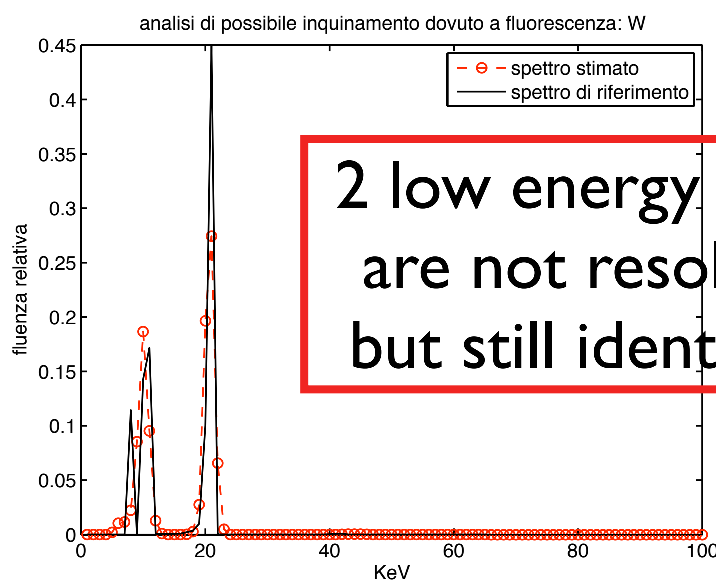
Thomson Source Simulations: pollution study



1 low energy peak is precisely identified

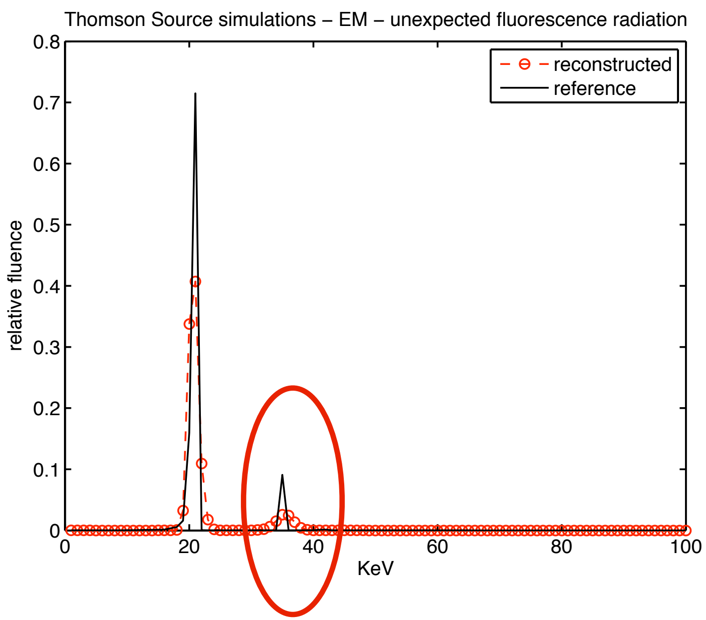


2 low energy peak are well recognized

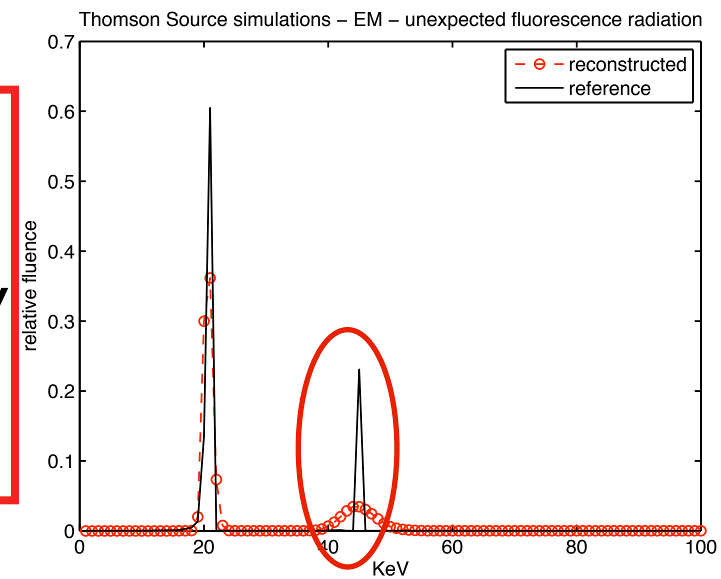


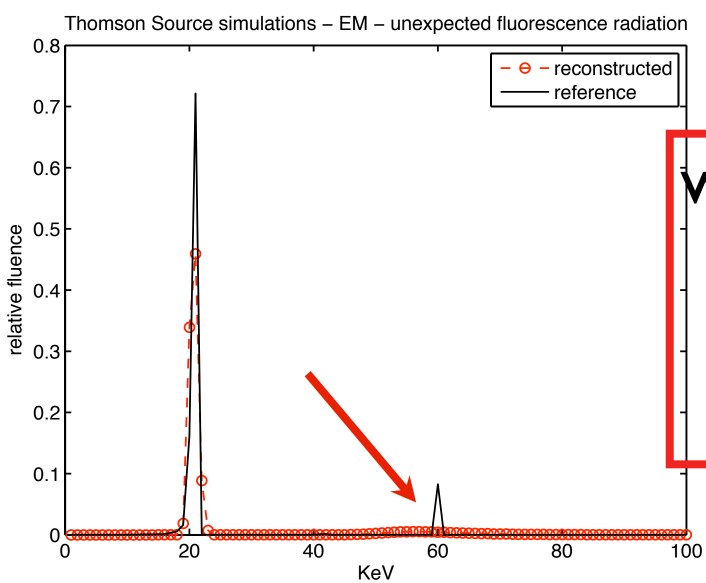
2 low energy peak are not resolved but still identified

Thomson Source Simulations: pollution study

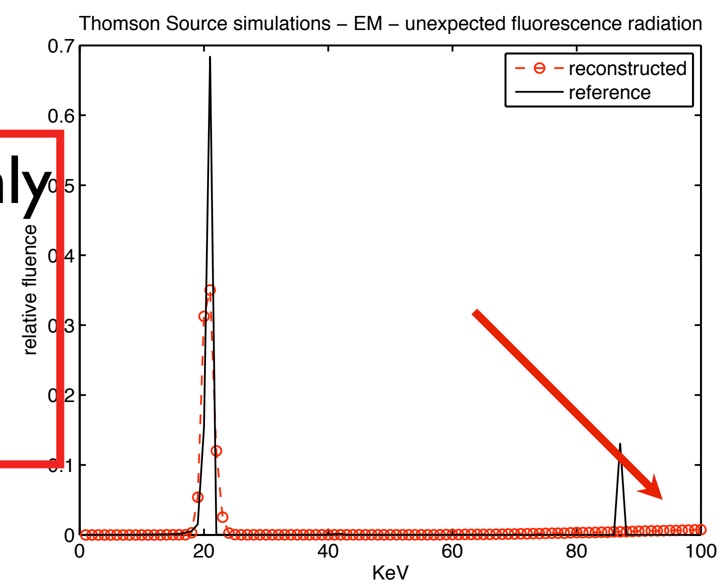


at least in terms of mean energy the line is identified





we can see only a very small unexpected variation



CONCLUSIONS

- a COMPLETE METHOD for spectral estimation from attenuation data analysis has been demonstrated both on SIMULATED and REAL EXPERIMENTS for filtered Bremsstrahlung Xray radiation

- SIMULATION STUDIES seems to show that Expectation Maximization Algorithm can be useful in the characterization of a high fluence, quasi-monochromatic Xray source as ICS Sources can be

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- a COMPLETE METHOD for spectral estimation from attenuation data analysis has been demonstrated both on SIMULATED and REAL EXPERIMENTS for filtered Bremsstrahlung Xray radiation
- SIMULATION STUDIES seems to show that Expectation Maximization Algorithm can be useful in the characterization of a high fluence, quasi-monochromatic Xray source as ICS Sources can be

WAITING FOR A REAL ICS MEASUREMENTS

- evaluation of Tikhonov-type Regularization imposing flatness at the boundaries and using different norms (L1)
- simulation study of different stopping rules for Expectation Maximization Algorithm

- a different approach to this kind of indirect spectrometry
- for example DIFFRACTION and COMPTON SCATTERING measurements can be a good choice

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thank you