

Appendix 1

In this appendix, we give a brief introduction to the mathematical tools used throughout the article. Namely, the EKF, which is the main retrieval tool for the tomography problem, and the EM framework which allows to use a reduced model (in a broad sense) instead of the more appropriate one for the problem to be solved.

Extended Kalman filter

The EKF⁴⁵ is a technique for state-estimation in observation-evolution problems. It is a non-linear extension to the linear Kalman Filter,³¹ which has been used, for example, in estimation of physiological parameters.¹⁵ It was also employed to perform optical tomography on phantoms with good results.⁷ Considering a state-evolution model written in the form

$$x_{t+1} = F(x_t, u_t) + \eta_t, \quad \eta_t \sim N(0, Q_t) \quad (8)$$

$$y_{t+1} = G(x_t, u_t) + v_t, \quad v_t \sim N(0, R_t) \quad (9)$$

where F is the state-transition operator, G is the observation operator, η_t and v_t are noise terms following a Normal distribution $N(0, X)$ with mean 0 and covariance matrix X and u_t is a control variable. In this work, we used the state-transition operator as:

$$x_{t+1} = F(x_t) = x_t + \delta x$$

$$x_t = \begin{pmatrix} \mu_{a,t} \\ \mu_{s,t}' \end{pmatrix}$$

$$\mu_{a,t+1} = \mu_{a,t} + \delta\mu_a$$

$$\mu_{s,t+1}' = \mu_{s,t}' + \delta\mu_s'$$

and the measurement is the observation operator. The EKF uses a linearization of the non-linear operators F and G , and it is suitable for problems with weak non-linearities. The covariance matrices Q_t and R_t are the process and measurement covariances, respectively. They determine the uncertainty of the current estimate x_t and y_t . The method consists of two steps: the prediction step, where the unknown x_{t+1} evolves according to the transition operator F , and the updating step, where the update is performed according to the predicted state and corrected by the observation operator G . The entire process contemplates the presence of additive

Gaussian noise in the evolution as well as in the measurement. The expressions for the predict and update equations for step $t \geq 1$ are given by²⁹:

Predict step :

$$x_{t+1|t} = F(x_{t|t}) + Q_t$$

$$\Gamma_{t+1|t} = F'_t \Gamma_{t|t} (F'_t)^T$$

Update step :

$$K_t = \Gamma_{t+1|t} H'_t (H'_t \Gamma_{t+1|t} (H'_t)^T + R_t)^{-1}$$

$$x_{t+1|t+1} = x_{t+1|t} + K_t [y_t - H(x_{t+1|t})]$$

$$\Gamma_{k+1|k+1} = (I - K_t H'_t) \Gamma_{t+1|t}$$

where $F'_t = \frac{\partial F}{\partial x}(x_{t|t})$, $H'_t = \frac{\partial G}{\partial x}(x_{t+1|t})$ and Γ is the evolution covariance matrix, which evolves by

accumulating information of prior steps given that the evolution relates the transition and observation operators (specifically, linearizations of them). The subscript $*|t$ is reserved for variables in the prediction step, while the subscript $*|t+1$ is used for variables in the update step.

Error modeling

The EM approach lies in the replacement of a given model A , which can represent correctly a given situation, for another model A_h which can be a simplification or a model which does not work as well as the first^{30,35,47}

In this way, we can use A_h in replacement of A by performing the following calculation:

$$A(x) = A_h(x) + [A(x) - A_h(x)]$$

$$A(x) = A_h(x) + \varepsilon(x)$$

where $\varepsilon(x)$ is defined as the modeling error. By creating samples and evaluating them using both models, it is possible to construct an empirical approximation to the EM distribution. Precisely, let l be the sample size,

and $S = \{x^{(1)}, \dots, x^{(l)}\}$ be the sample. Then, we evaluate them using both models and constructing an array of EM with the i th element defined as

$$E_i = A(x^{(i)}) - A_h(x^{(i)}).$$

The true EM distribution can be estimated and used. However, if the sample allows it, it is possible to use a Normal approximation to the EM distribution. In order to add this information to the EKF, we subtract the mean of the EM e_0 as well as add the empirical covariance of the sample Γ_{x_h} to the parameter covariance, and adding the empirical covariance of the EM Γ_H to the measurement covariance R , i.e.

$$\begin{aligned}\hat{y}_0 &= \hat{y} - e_0 \\ \Gamma_0 &= \Gamma_0 + \Gamma_{x_h} \\ R_t &= R_t + \Gamma_H\end{aligned}$$

In this work, samples containing only spherical inclusions were used. This can be seen as a form of (soft) prior information because the error mean and covariance were calculated using those samples. In Figure 9, a comparison between the simulation and the retrieval processes can be seen. The output of the simulations is used to feed the retrieval algorithm. Please note that even though the inclusions in the simulations are well defined (spheres), during the retrieval process, no geometrical information is supplied to the EKF. The EM approach may introduce a bias if a non-zero mean e_0 is obtained, thus suggesting that in situations where the approximated model works properly, the corrected one may be biased, lowering precision, resolution, etc. Finally, for complex shaped non-scattering region,³ the DA-EM methodology is suitable. However, the sample generation should be modified using Gaussian smoothness prior⁷ instead of an ensemble of spheres. This prior generates complex random samples, resulting in better resolution and specificity of the retrieval process.

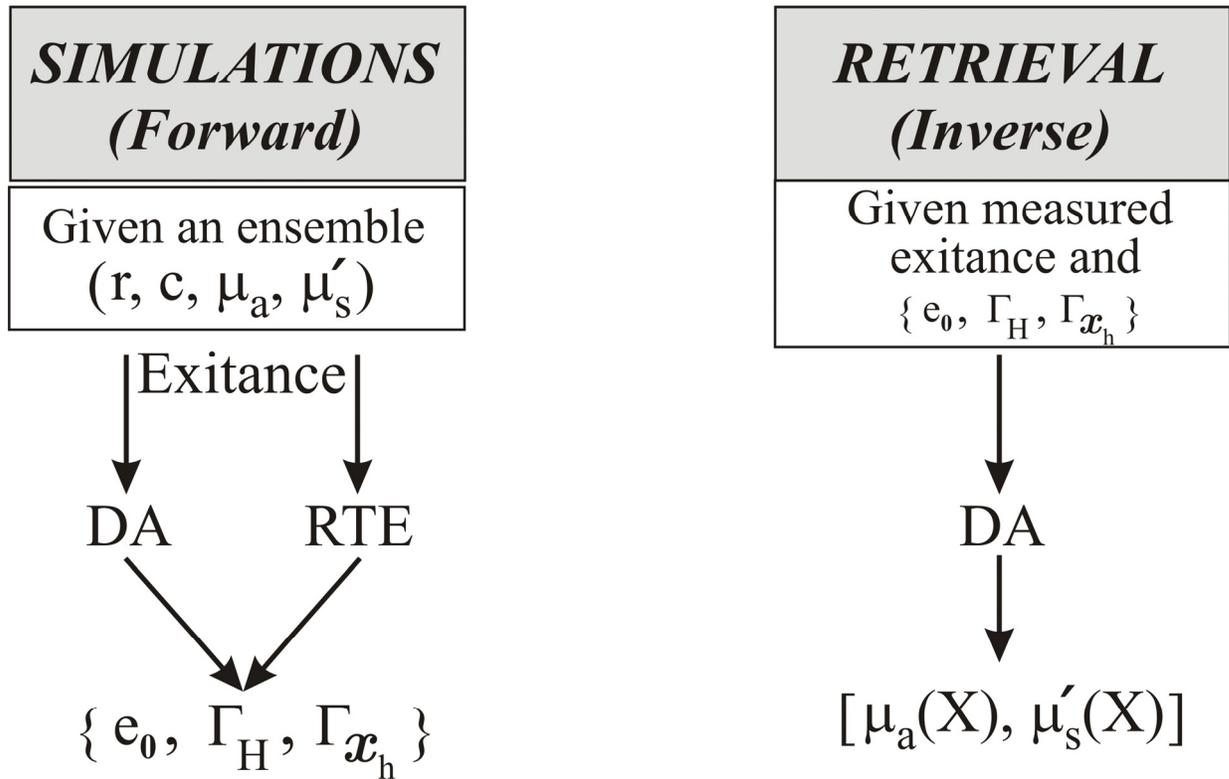


Figure 9. Scheme of the phases of the retrieval process. Left: an ensemble of simulations is performed for different (random) spherical inclusions. To this end, the inclusion radius (r), its center location (c), and their optical properties μ_a and μ'_s are drawn. The optical properties of the background are kept constant. The outputs of the simulations are the exitances for both DA and RTE. Finally, the mean error modeling (e_0), the error measurement covariance (Γ_H), and the sample covariance (Γ_{x_h}) are calculated. Right: an estimation of the optical properties is calculated for each node in the domain. To accomplish this operation, the objective measured exitance, (e_0), (Γ_H), (Γ_{x_h}) and the DA are used in the EKF machinery, as explained above. DA: diffusion approximation; RTE: radiative transfer equation.