Retrieval of ice crystal size related mass from IWC and PSD measurements: a numerical optimization approach

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MOTIVATION

Studies related to ice clouds often use the Particle Size Distribution (***PSD***) and Ice Water Content (***IWC***) to derive mass-size relationships [1], [2]. Crystals are sorted in size bins forming the PSD, whereas IWC constitutes the bulk measurement of the corresponding total mass of ice per volume of air. In most methods used to compute individual ice crystal mass from size, shape, and bulk information such as IWC or radar reflectivity [3] a power law is assumed. The coefficients of the mass-size relationship are then derived from fits of experimental data points and constrained by in-situ bulk measurements.

In the following, we present a ***new approach for the retrieval of ice crystal masses*** from PSD and IWC without presuming a particular form for the mass-size relationship. The method searches for the entire PSD the specific masses of crystals sorted in sufficiently narrow size bins. The mass vector is computed by ***solving*** an ***inverse*** ill-conditioned ***problem*** with ***numerical optimization techniques***.

METHODOLOGY

Problem statement:

Inverse problem ***(1)*** and objective function to be minimized ***(2)*** :

$$PSD.\boldsymbol{m} = \boldsymbol{IWC} \qquad (1)$$

$$J(\boldsymbol{m}) \stackrel{\text{def}}{=} \|PSD.\boldsymbol{m} - \boldsymbol{IWC}\|^2 + \lambda . R(\boldsymbol{m}) \qquad (2)$$

With $\boldsymbol{m}$ the mass solution vector of the bin resolved problem ***(1)***

- PSD matrix of Particle Size Distribution
- $\boldsymbol{IWC}$ vector of IWC values
- $\lambda \in \mathbb{R}^{*+}$ regularization parameter
- $R(\boldsymbol{m})$ regularization function

Minimization algorithms [4] :

The minimization is performed using iterative algorithms :

- move from one iterate to the next : ***Line Search*** approach

$$\boldsymbol{m^{k+1}} = \boldsymbol{m^k} + \alpha^k \cdot \boldsymbol{p^k}$$

- search direction : $\boldsymbol{p^k}$ ***inexact Newton-CG*** method
- step length : $\alpha^k = 1$ or ***Backtracking Line Search*** scheme

Optimization parameters:

- λ optimal determination: ***L-curve*** technique
- regularization : enforce curve smoothness [5]

$$R(\boldsymbol{m}) = \|D \cdot \boldsymbol{m}\|^2, \quad D \stackrel{\text{def}}{=} \begin{bmatrix} D_{i,j} = s_i, \text{for } i = j \\ D_{i,j} = -s_i, \text{for } i = j+1 \\ 0 \text{ elsewhere} \end{bmatrix}, \quad s_i = \frac{1}{\pi/6 \cdot \rho \cdot (d_{bin} + 50)^3}$$

Validation of the proposed method:

Robustness and performance are assessed using synthetic crystal populations:

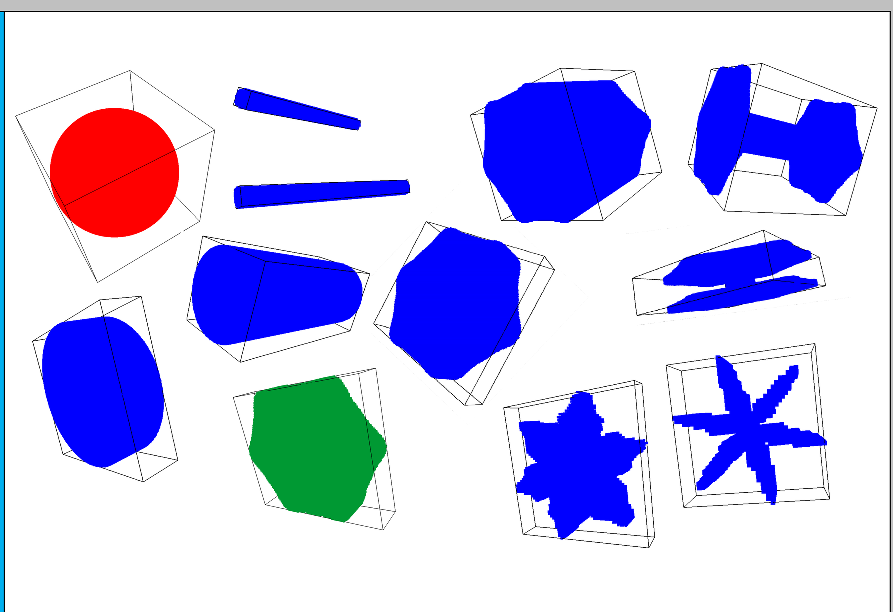
- known 3D geometry and mass
- possibility to gradually increase data noise (due to loss of information during 2D projections of 3D volume mainly)

Validation of optimization results:

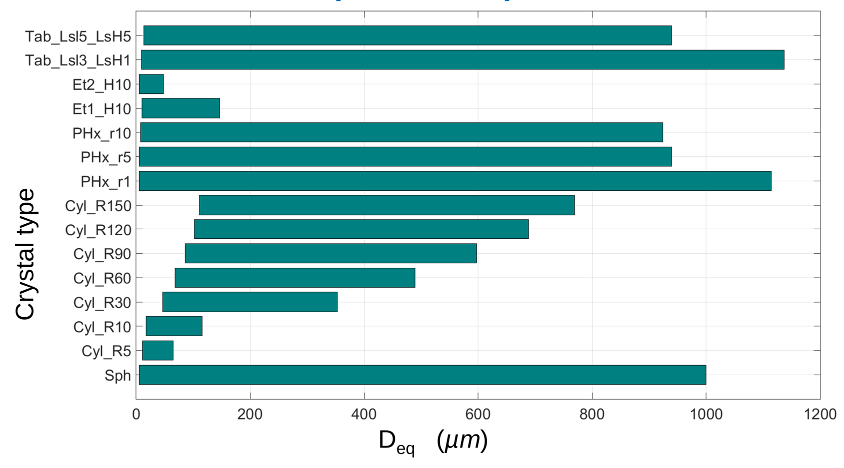
3 different synthetic crystal populations following a normal distribution law (mean = μ , standard deviation = σ) are generated:

- sub-dataset n°1: ($\mu = 300\ \mu m$), used to perform the optimization and compute the mass solution
- Sub-dataset n°2, n°3 : ($\mu = 100, 600\ \mu m$, respectively), used to validate the mass vector retrieved from sub-dataset n°1

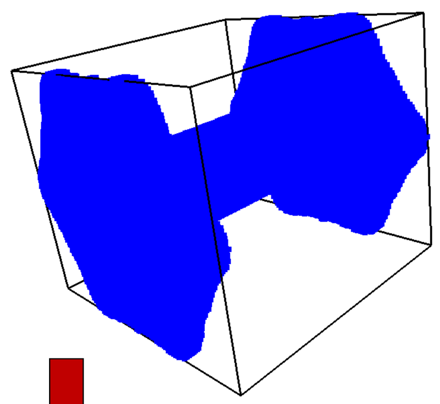
Synthetic crystal dataset



- ***various*** geometrical ***shapes***
- sizes from ***15 µm*** to ***1000 µm***

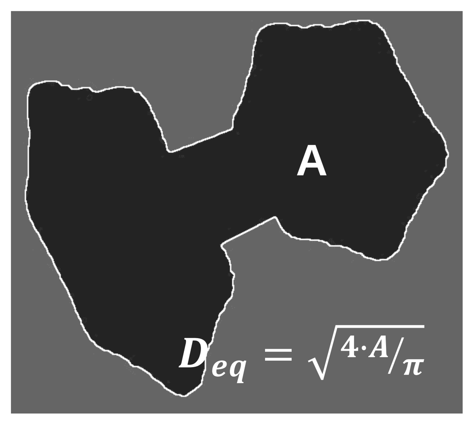


1 - Randomly oriented Volume



Projection of 3D volume

2 - Projected Area

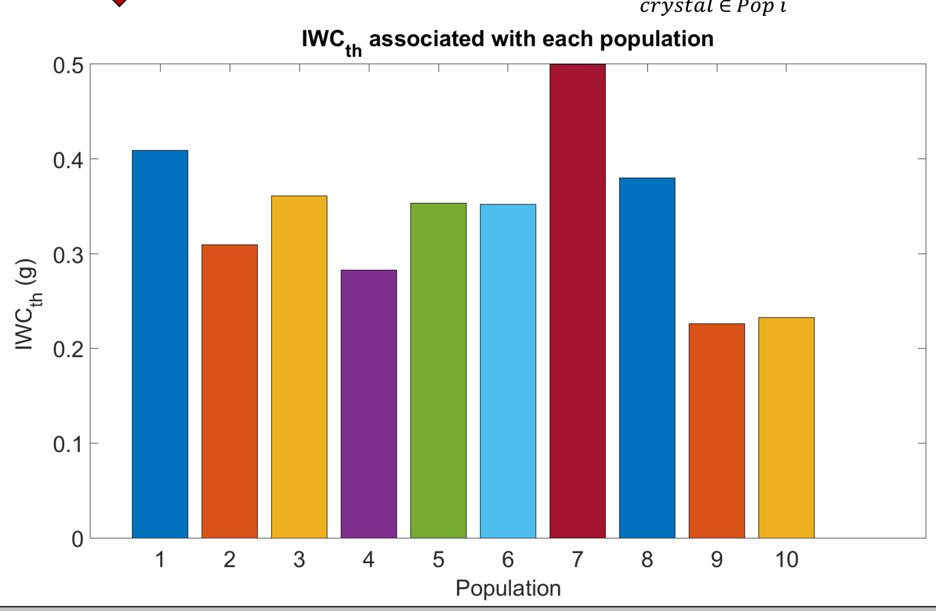


2D image analysis

3 - Tables of Geometric parameters

Volume	Area	Deq
87451	2135	52
87451	3150	63
93093	2919	61
93093	1953	50
98735	2913	61
98735	2479	56
104377	2799	60
104377	3576	67

$$m_{crystal} = \rho \cdot V_{crystal} \quad \& \quad IWC_i = \sum_{crystal \in Pop\ i} m_{crystal}$$

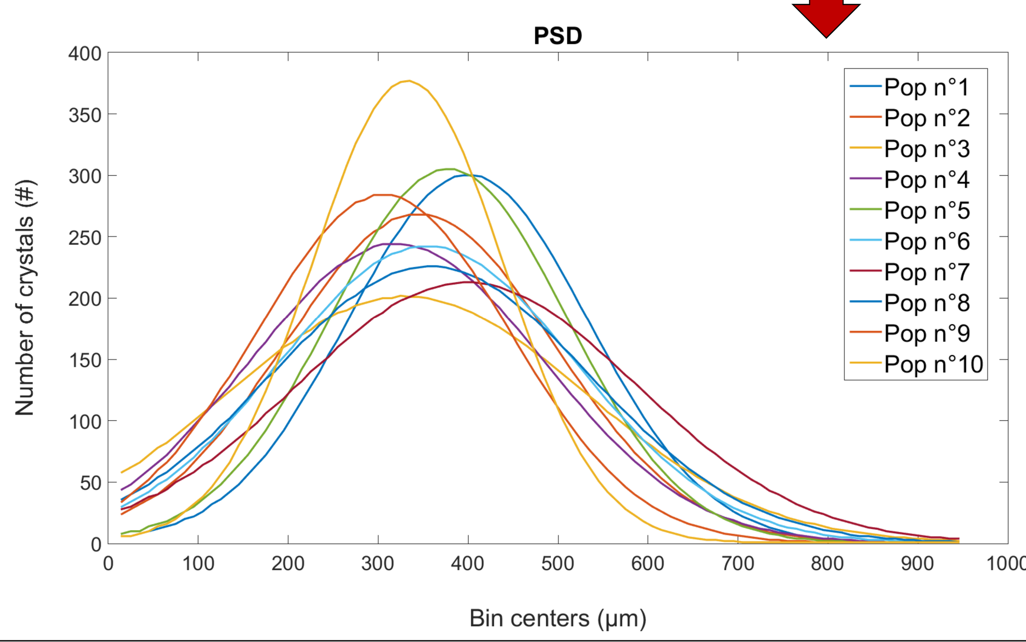


Example: Populations of crystals sorted in ***10 size bins***. To compute the crystal mass in each bin, we need at least 10 linearly independent subpopulations – i.e. ***10 pairs*** $(\boldsymbol{PSD}, \boldsymbol{IWC})$ from which the linear system is formed.

$$\begin{cases} IWC_1 = PSD_1 \cdot \boldsymbol{m} \\ IWC_2 = PSD_2 \cdot \boldsymbol{m} \\ \vdots \\ IWC_{10} = PSD_{10} \cdot \boldsymbol{m} \end{cases}$$

This can be written as a matrix equation as mentioned in ***(1)***.

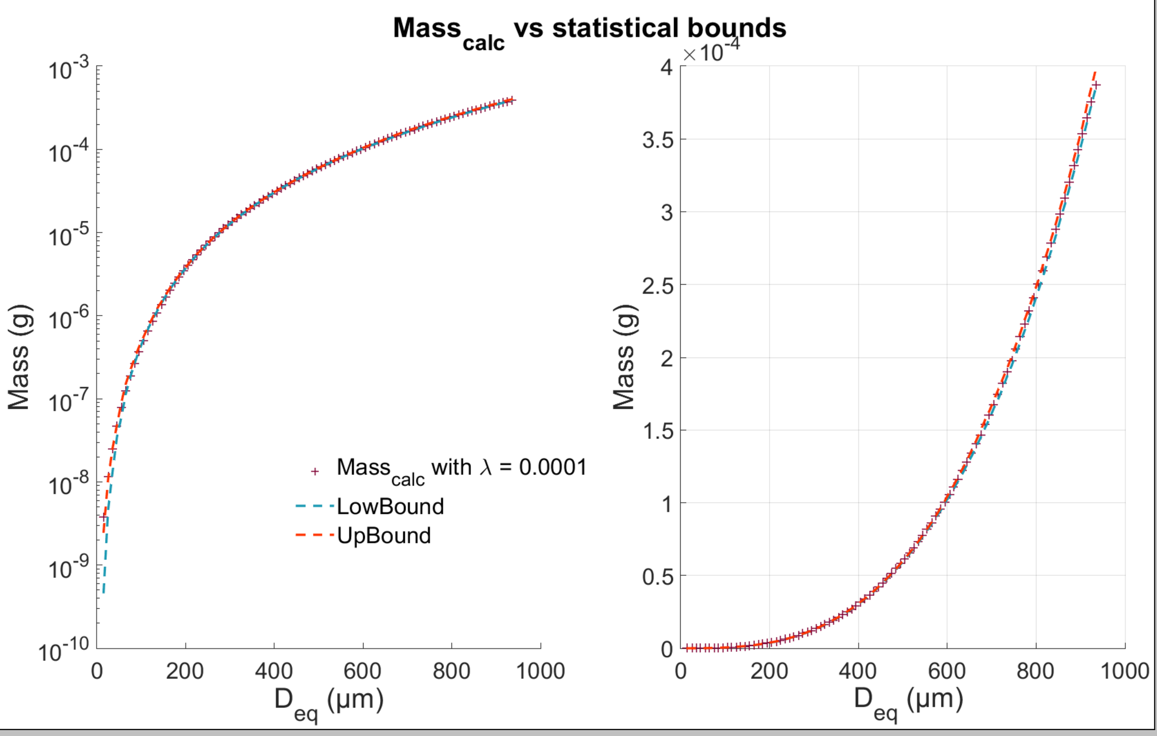
Normal distributions with various μ, σ values.

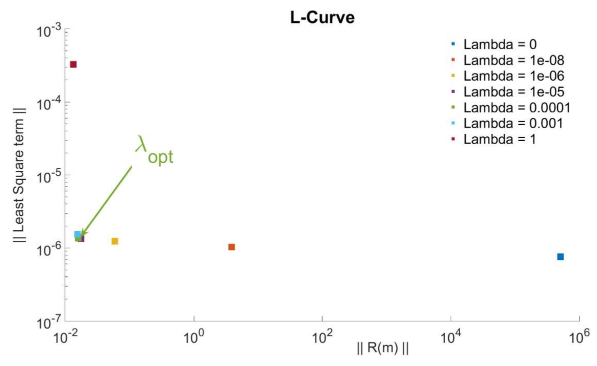


RESULTS

Case A: population of ***Spheres***

- $15 \leq d_{Sph} \leq 939\ \mu m$





Quality assessment of the solution:

$$\overline{MAER} = \frac{1}{N_{pop}} \sum_{N_{pop}} \frac{|IWC_{calc} - IWC_{th}|}{IWC_{th}}$$

with

$IWC_{calc} = \boldsymbol{PSD_v} \cdot \boldsymbol{m_{sol}}$

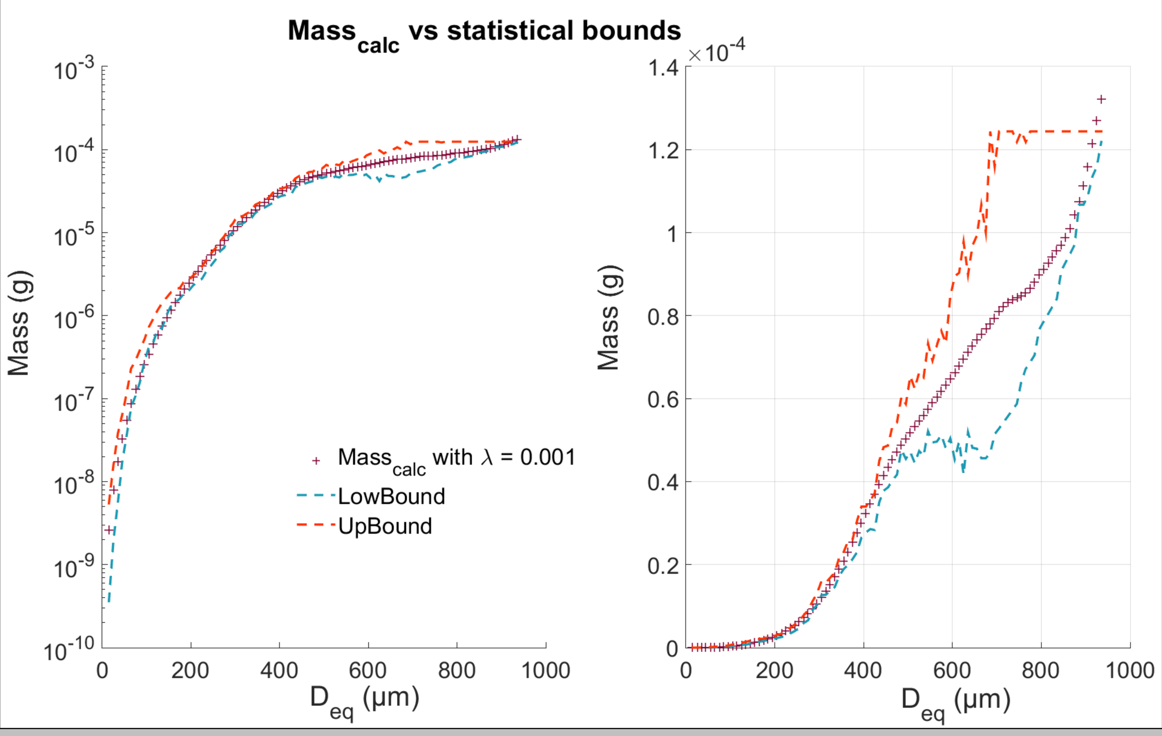
$\boldsymbol{PSD_v}$ & IWC_{calc} from dataset n°2 or 3

Highlights:

- ***good agreement with expected mass variations,*** even for crystals with poor 3D symmetry.
- The ***solution lies inside the statistical bounds*** obtained from crystals' theoretical masses
- Computations of IWC from PSDs of dataset n°2/3 and from the solution vector obtained from dataset n°1 yield very consistent results: ***Mean Absolute Relative Error on IWC*** averaged over 186 data points is ***less than 1%*** !

Case B: population of ***Hexagonal Plates***

- $15 \leq d_{PHx} \leq 939\ \mu m$, $length/thickness = 5$



CONCLUSIONS & PERSPECTIVES

The ***method*** proves to be ***very promising*** : results based on low complexity synthetic datasets reveal very good ability to retrieve masses that fit experimental data while allowing the use of potential prior knowledge via the regularization term. Computation time for PSD ranging from 15 to 935 μm (93 size bins of 10μm width) is in the order of a few tens of seconds.

Upcoming work will focus on:

- ***Increasing the synthetic dataset complexity*** by allowing more realistic crystal geometries (*e.g.* aggregates of ice crystals, inclusion of air in capillary spaces)
- ***Identifying prior information*** with respect to ***ice crystal microphysics*** that could be used to improve minimization results and define a regularization function accordingly
- ***Applying the method to HAIC/HIWC flight campaign datasets*** (1284 size bins of 10μm width) and assess the quality of mass retrieval from in-situ measurements dataset

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