A New Algorithm for Computing the Radial Distribution Function in Three-Dimensional Measurement Volumes

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INTRODUCTION/ATMOSPHERIC CONTEXT

Quantifying cloud particle clustering is important to help develop and verify theories associated with condensational growth, collision-coalescence, radiative transfer, and aircraft icing. One of the more common statistical tools used to characterize this clustering is the radial distribution function (hereafter rdf or g(r)).

Most previous studies that have attempted to estimate the *in situ* radial distribution function among cloud droplets utilize data obtained from a long but thin sample volume, resulting in cloud droplet positions recorded only along a single spatial dimension. Although it is theoretically possible to take such one-dimensional data and estimate three-dimensional radial distribution functions, recent studies have shown that (i) such approaches rely on questionable assumptions related to statistical homogeneity and isotropy on large (>100m) spatial scales and (ii) sampling uncertainties related to such one-dimensional data can yield considerable uncertainties in the inferred three-dimensional rdf.

Fortunately, digital holographic instruments have been recently developed that allow for full three-dimensional measurement of cloud droplet positions. Utilizing data from these instruments should allow for a more robust estimate of *in situ* cloud particle clustering. However, estimating the rdf within a finite three-dimensional sample volume brings about new challenges.

THE RADIAL DISTRIBUTION FUNCTION

The radial distribution function [g(r)] is a statistical tool that supplies a scale-localized deviation from perfect spatial randomness. Conceptually, we can write:

$g(r_0) =$
$\dfrac{\text{[Observed number of particle pair centers separated by } (r_0-dr<r<r_0+dr)]}{\text{[Expected \# of particle pair centers separated by } (r_0-dr<r<r_0+dr) \text{ if perfectly random]}}$

When $g(r_0)=1$, this implies that on scale r_0 there are no departures from perfect spatial randomness. When $g(r_0)$ exceeds unity, it shows that particle pairs are more likely than expected to be separated by spatial scale r_0.

To compute g(r) for a measured data set, we can write:

$$g(r) = \sum_{i=1}^{N} \frac{\psi_i(r)/N}{(N-1)\left(\frac{\mathrm{d}V_r}{V}\right)}$$

where N is the number of particles in the measurement volume, V is the size of the measurement volume, dV_r is the volume of the generalized n-dimensional shell between radii r-dr and r+dr, and $\psi_i(r)$ is the number of particles having their centers a distance between r-dr and r+dr from the center of the ith particle.

CHALLENGES IN COMPUTING THE RDF IN 3-D
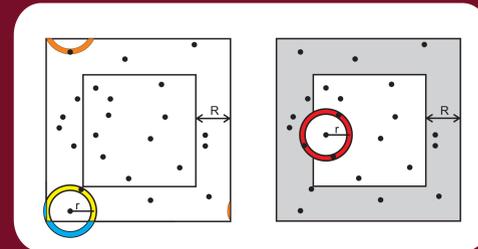
The biggest challenge in computing the radial distribution functions for finite volumes in 2+ dimensions relates to how to handle the edges of the sample volume. Numerical studies often utilize periodic boundary conditions to compute g(r), but this is not physically meaningful for measurement volumes. An alternative approach used is to exclude a boundary region (see grey areas in figures to left), but this excludes large fractions of the observational data, especially in three-dimensional data-sets and/or when the measurement volume has a large aspect ratio.
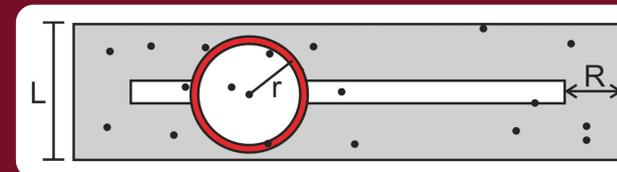
In fact, the "excluded-volume" method prevents any estimate of g(r) for scales larger than L/2, where L is the length of the shortest dimension of the sample volume. Given the aspect ratios associated with real instrumentation (see example below from HOLODEC – the holographic detector for clouds), this would severely limit our ability to characterize cloud particle clustering and prevent estimating g(r) on scales greater than 3 mm.

HOLODEC

2D Cartoon of HOLODEC measurement volume
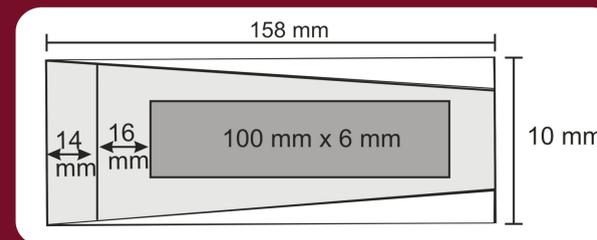
DESCRIPTION OF ALGORITHM

$dV_{r(i,j)}=[12/(12+16)] \, dV_r$

Here, we introduce a new "effective-volume" algorithm. We modify g(r) to read:

$$g(r_j) = \sum_{i=1}^{N} \frac{\psi_i(r_j)/N}{(N-1)\left(\frac{\mathrm{d}V_{r_{i,j}}}{V}\right)}$$

where we have modified the dV_r term to be the volume in the generalized n-dimensional shell between radii r-dr and r+dr still residing within the measurement volume. This is computed using the volume of the full n-dimensional shell and then multiplying by a look-up-table estimate based on r, dr, and the position within the sample volume.
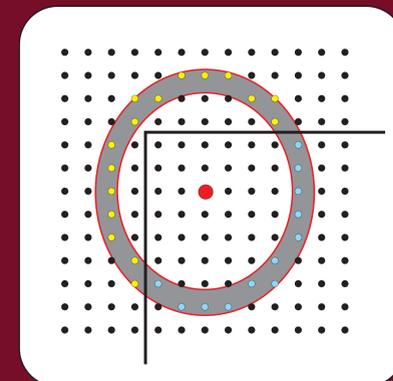
TESTING THE ALGORITHM

Cubical Geometry
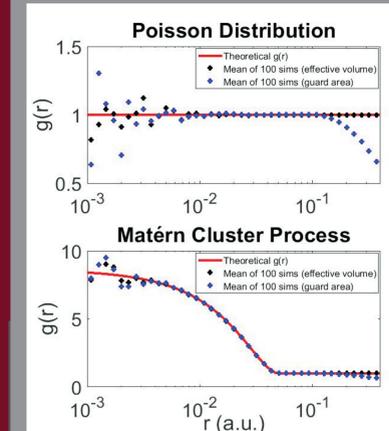
The "effective-volume" algorithm was tested against the theoretically known rdf for two different systems within a unit cube – a Poisson pdf (where g(r) should be unity for all scales) and a Matérn cluster process (where g(r) has a known analytical form). The effective-volume method performed as well or better than the previously utilized excluded volume method in these tests.

10 cm x 6 mm x 6 mm

The "effective-volume" algorithm was tested against the same two theoretically known rdf curves in a sample volume designed to mimic the HOLODEC sample volume. There is still excellent agreement. The excluded volume method cannot be used for this sample volume because of the HOLODEC measurement volume aspect ratio.
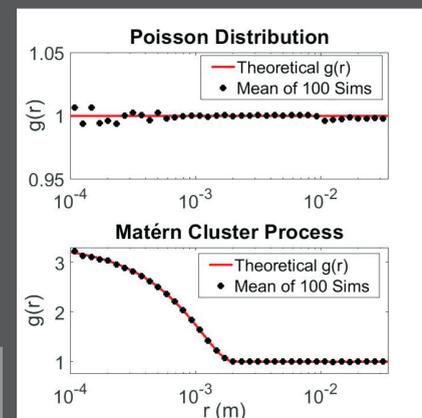
Practical utility is demonstrated by computing the rdf for real HOLODEC data taken inside a cloud chamber. Although sampling noise is substantial (and a subject of continuing study), retrieval of 3-D rdf curves appears possible.
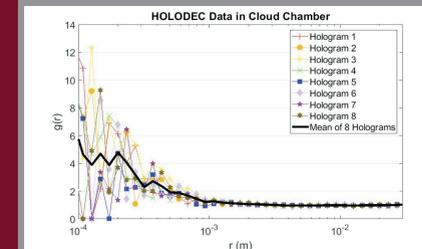
FURTHER READING

Larsen, M.L. and R.A. Shaw (2018). A Method for Computing the Three-Dimensional Radial Distribution Function of Cloud Particles from Holographic Images. *Atmospheric Measurement Techniques Discussion*, https://doi.org/10.5194/amt-2018-60, in review.

Ripley, B. (1982). Edge Effects in Spatial Stochastic Processes, in: Statistics in Theory and Practice: Essays in Honour of Bertil Matern. B. Ranneby, editor.

ACKNOWLEDGMENTS