SMRT Microstructure

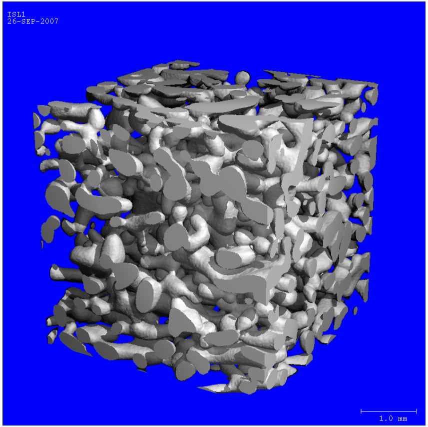
Henning Löwe

WSL Institute for Snow and Avalanche Research SLF, Davos, Switzerland

3rd SMRT Training School, AWI, 06-08 July 2023

Microstructure in SMRT

Snow microstructure as seen by X-ray tomography:



- A key driver for developing SMRT: Faithful representation of microstructure

Recap from EM lecture: Where microstructure matters

IBA phase function: (cf. yesterday)

$$p\left(\vartheta, \varphi\right)_{\text{1-2 frame}} = M(|\mathrm{k}_d|) k_0^4 \, \sin^2 \chi (\epsilon_2 - \epsilon_1)^2 \; Y^2(\epsilon_1, \epsilon_2) \quad (1)$$

- Angular distribution of scattered intensity

Recap from EM lecture: Where microstructure matters

IBA phase function: (cf. yesterday)

$$p\,(\vartheta,\varphi)_{\text{1-2 frame}} = M(|\mathrm{k}_d|)k_0^4\ \sin^2\chi(\epsilon_2-\epsilon_1)^2\ Y^2(\epsilon_1,\epsilon_2) \tag{1}$$

- Angular distribution of scattered intensity

Microstructure term

$$M(|\mathrm{k_d}|) = \frac{\widetilde{C}(|\mathrm{k}_d|)}{4\pi}. \tag{2}$$

- defined by the Fourier transform $\widetilde{C}(|\mathrm{k}_d|)$ of the auto-correlation function (ACF).

Recap from EM lecture: Where microstructure matters

IBA phase function: (cf. yesterday)

$$p\,(\vartheta,\varphi)_{\text{1-2 frame}} = M(|\mathsf{k}_d|)k_0^4\ \sin^2\chi(\epsilon_2-\epsilon_1)^2\ Y^2(\epsilon_1,\epsilon_2) \tag{1}$$

- Angular distribution of scattered intensity

Microstructure term

$$M(|\mathsf{k}_\mathsf{d}|) = \frac{\widetilde{C}(|\mathsf{k}_d|)}{4\pi}. \tag{2}$$

- defined by the Fourier transform $\widetilde{C}(|\mathsf{k}_d|)$ of the auto-correlation function (ACF).

Goal of the lecture

- Understand the ACF and its implications for scattering

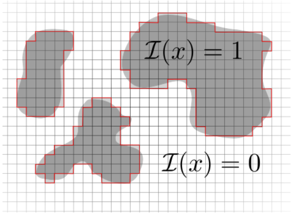
Outline

Definition of the ACF for random media

Indicator function of the ice phase:

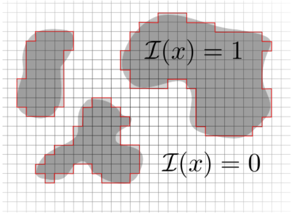
$$\mathcal{I}(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \boldsymbol{x} \text{ is in ice} \\ 0, & \text{if } \boldsymbol{x} \text{ is in air} \end{cases}$$

- A μCT image is a discrete version of it



Definition of the ACF for random media

Indicator function of the ice phase:



$$\mathcal{I}(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \boldsymbol{x} \text{ is in ice} \\ 0, & \text{if } \boldsymbol{x} \text{ is in air} \end{cases}$$

- A μCT image is a discrete version of it

Auto-correlation function (ACF) and Fourier transform (3D):

$$C(\boldsymbol{r}) = \overline{(\mathcal{I}(\boldsymbol{x}) - f_2)(\mathcal{I}(\boldsymbol{x}+\boldsymbol{r}) - f_2)}$$

$$\widetilde{C}(\boldsymbol{k}) = \int d\boldsymbol{r} \exp(-i\boldsymbol{r}\cdot\boldsymbol{k})C(\boldsymbol{r})$$

- Spectrum of (micro-scale) density fluctuations
- SMRT involves only $\widetilde{C}(|\boldsymbol{k}|)$ (isotropy)

Basic geometrical properties of the ACF:

Special values and geometrical meaning:

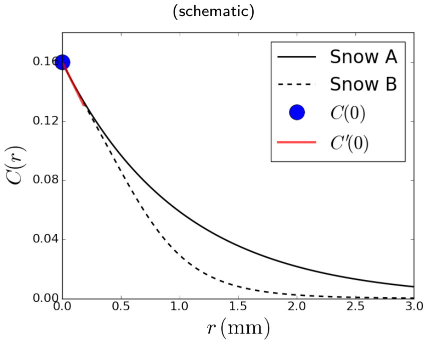
- Link to density:

$$C(0) = f_2(1 - f_2)$$

- Link to specific surface area (SSA):

$$C'(0) = 1/\ell_p = \frac{\mathrm{SSA}\,\rho_{\mathrm{ice}} f_2}{4}$$

ℓ_p: Porod length, f_2: ice volume fraction



Basic geometrical properties of the ACF:

Special values and geometrical meaning:

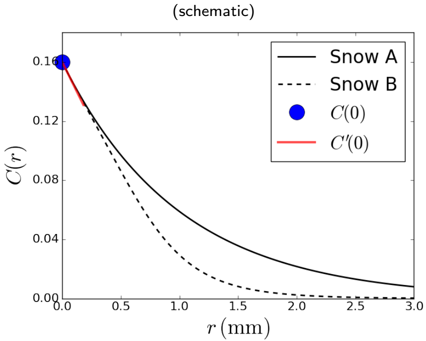
- Link to density:

$$C(0) = f_2(1 - f_2)$$

- Link to specific surface area (SSA):

$$C'(0) = 1/\ell_p = \frac{\mathrm{SSA}\,\rho_{\mathrm{ice}} f_2}{4}$$

ℓ_p: Porod length, f_2: ice volume fraction



Implication:

- Density and SSA characterize only the behavior of $C(r \approx 0)$
- Density and SSA not sufficient to characterize MW scattering

From μCT images to SMRT simulations

Computing the ACF for a 3d image:

- $C(\boldsymbol{r})$ is a discrete convolution of the image with itself (N voxels)

$$
\begin{aligned}
C(\boldsymbol{r}) &= \overline{(\mathcal{I}(\boldsymbol{x}) - f_2)(\mathcal{I}(\boldsymbol{x}+\boldsymbol{r}) - f_2)} \\
&\approx \frac{1}{V}\int d\boldsymbol{x}\, (\mathcal{I}(\boldsymbol{x}) - f_2)(\mathcal{I}(\boldsymbol{x}+\boldsymbol{r}) - f_2) \\
&\approx \frac{1}{N} (\mathcal{I}(\boldsymbol{x}) - f_2) * (\mathcal{I}(\boldsymbol{x}+\boldsymbol{r}) - f_2) \\
&\approx \frac{1}{N} \mathcal{F}^{-1} \parallel \mathcal{F}[\mathcal{I}(\boldsymbol{x}) - f_2] \parallel^2
\end{aligned}
$$

From μCT images to SMRT simulations

Computing the ACF for a 3d image:

- $C(\boldsymbol{r})$ is a discrete convolution of the image with itself (N voxels)

$$
\begin{aligned}
C(\boldsymbol{r}) &= \overline{(\mathcal{I}(\boldsymbol{x}) - f_2)(\mathcal{I}(\boldsymbol{x}+\boldsymbol{r}) - f_2)} \\
&\approx \frac{1}{V}\int d\boldsymbol{x}\, (\mathcal{I}(\boldsymbol{x}) - f_2)(\mathcal{I}(\boldsymbol{x}+\boldsymbol{r}) - f_2) \\
&\approx \frac{1}{N} (\mathcal{I}(\boldsymbol{x}) - f_2) * (\mathcal{I}(\boldsymbol{x}+\boldsymbol{r}) - f_2) \\
&\approx \frac{1}{N} \mathcal{F}^{-1} \parallel \mathcal{F}[\mathcal{I}(\boldsymbol{x}) - f_2] \parallel^2
\end{aligned}
$$

Fitting $C(\boldsymbol{r})$ to an ACF model:

- Yields parameters to initialize SMRT microstructure (=Parametric ACF model)
- Parametric ACF models required for the numerics

ACF models available in SMRT

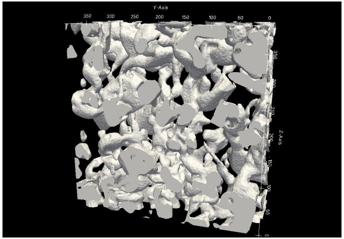
(`smrt.microstructure`)

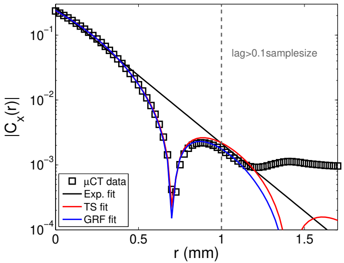
Model	Origin	# Param's	Defined by
Exponential	MEMLS	1	$A_{\mathrm{ex}}(r) = \exp(-r/l_{\mathrm{ex}})$
Teubner–Strey	Microemulsions	2	$A_{\mathrm{TS}}(r) = \exp(-r/\xi_{\mathrm{TS}}) \frac{\sin(2\pi r/d_{\mathrm{TS}})}{(2\pi r/d_{\mathrm{TS}})}$
Independent sphere	Sparse media	1	a *spherical* ACF
Sticky hard spheres	QCA/DMRT	2	(later)
Gaussian random field	3D reconstruction	2	an auxiliary ACF
Unified models	[Picard et al 2022]	2	(later)

where $C(r) = C(0)A(r)$.

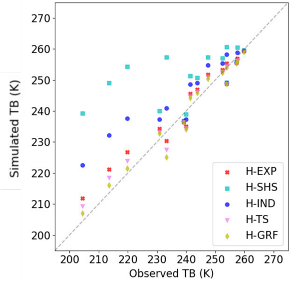
Comparison of different ACF models

Fitting the same image to different ACF models:





- Clear difference in performance
- EXP less flexible than TS (evident)
- Profound impact on MW modeling (cf. right)
- More on this → practical

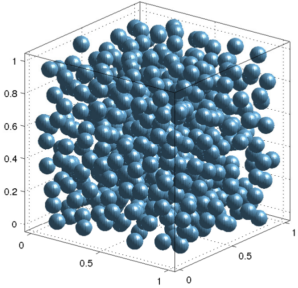


[Sandells et al, IEEE TGRS, 2022]

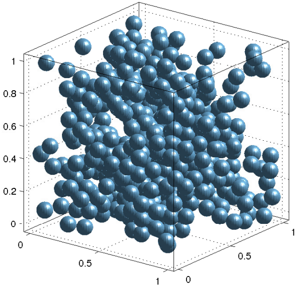
Outline

Sticky hard spheres: The basis of QCA and DMRT

- Determined by volume fraction f_2, diameter d, and stickiness τ [Baxter, 1967]
- Example realizations (identical f_2, d, i.e. same SSA):



$\tau = 10.0$



$\tau = 0.11$

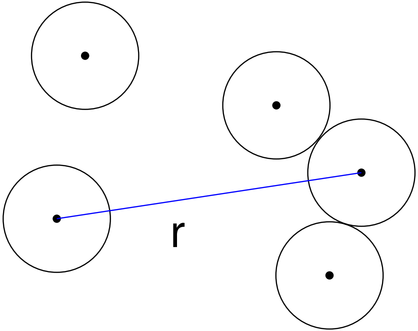
Main effect of stickiness τ:

- Clustering $\rightarrow$ new structural length scales $\rightarrow$ impact on scattering

How can sphere models be related to $C(r)$?

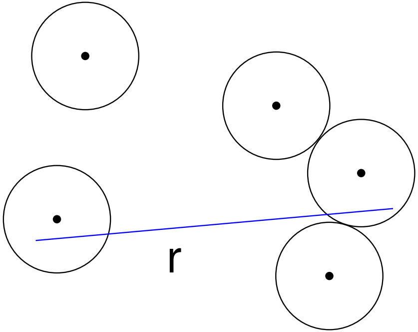
Commonly formulated in different types of correlation functions:

DMRT is based on:



Pair correlation function: $g(\boldsymbol{r})$
($\rightarrow$ Prob. that $\boldsymbol{r}$ connects the *centers* of two spheres)

IBA requires:



Two-point correlation function: $C(\boldsymbol{r})$
($\rightarrow$ Prob. that $\boldsymbol{r}$ connects the *interior* of two spheres

Relating two-point correlations and pair correlations:

Exact result for arbitrary (hard) sphere packings:

$$C(\boldsymbol{r}) = n v_{\mathrm{int}}(\boldsymbol{r}) + n^2 \left(v_{\mathrm{int}} * g \right)(\boldsymbol{r})$$

- $v_{\mathrm{int}}(\boldsymbol{r})$: Intersection volume of two spheres, n: number density of spheres

Relating two-point correlations and pair correlations:

Exact result for arbitrary (hard) sphere packings:

$$C(\boldsymbol{r}) = n v_{\mathrm{int}}(\boldsymbol{r}) + n^2 \left(v_{\mathrm{int}} * g\right)(\boldsymbol{r})$$

- $v_{\mathrm{int}}(\boldsymbol{r})$: Intersection volume of two spheres, n: number density of spheres

Equivalent in Fourier space:

$$\widetilde{C}(\boldsymbol{k}) = nP(\boldsymbol{k})S(\boldsymbol{k})$$

- $P(\boldsymbol{k})$: form factor, $S(\boldsymbol{k})$: structure factor [Stell & Torquato 1982]

Relating two-point correlations and pair correlations:

Exact result for arbitrary (hard) sphere packings:

$$C(\boldsymbol{r}) = n v_{\mathrm{int}}(\boldsymbol{r}) + n^2 \left(v_{\mathrm{int}} * g\right)(\boldsymbol{r})$$

- $v_{\mathrm{int}}(\boldsymbol{r})$: Intersection volume of two spheres, n: number density of spheres

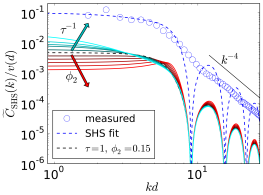
Equivalent in Fourier space:

$$\widetilde{C}(\boldsymbol{k}) = n P(\boldsymbol{k}) S(\boldsymbol{k})$$

- $P(\boldsymbol{k})$: form factor, $S(\boldsymbol{k})$: structure factor [Stell & Torquato 1982]

This link allows to:

- implement DMRT's sticky hard spheres in IBA
- compare QCA scattering formulations with IBA
- fit μCT images to sticky hard spheres (not worth it)



[Löwe & Picard, TC, 2015]

Comparison of IBA and QCA-CP

Scattering coefficient κ_s (low freq):

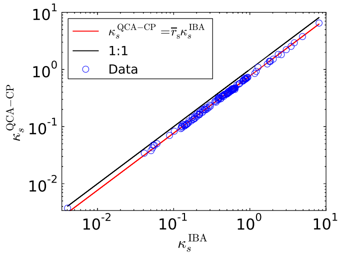
$$\kappa_s^{\mathrm{IBA}} = \frac{2}{9} k_0^4 a^3 \phi_2 f^{\mathrm{IBA}}(\varepsilon_1, \varepsilon_2, \phi_2)\, \widetilde{C}(0)$$

$$\kappa_s^{\mathrm{QCA-CP}} = \frac{2}{9} k_0^4 a^3 \phi_2 f^{\mathrm{QCA-CP}}(\varepsilon_1, \varepsilon_2, \phi_2)\, \widetilde{C}(0)$$

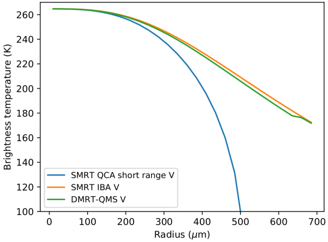
- Same microstructure term $\widetilde{C}(0)$

Main message:

- IBA $\approx$ QCA-CP (shortrange) for low frequency
- IBA $\approx$ QCA (longrange) for higher frequency



[Löwe & Picard, TC, 2015]



[Picard et al, TC, 2018]

Outline

Motivation

ACF: Definition and properties

ACF for spheres: Linking IBA and QCA

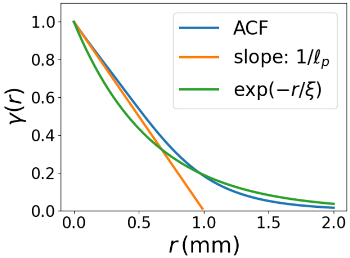
ACF reinterpreted: The microwave grain size

What if we dont't have ACF measurements?

Snow field measurements:

- Often no μCT $\Rightarrow$ no ACF
- Always SSA estimates
  (DUFISS, IRIS, IceCube, SMP, InfraSnow, ...)

What if we dont't have ACF measurements?



Snow field measurements:

- Often no μCT $\Rightarrow$ no ACF
- Always SSA estimates (DUFISS, IRIS, IceCube, SMP, InfraSnow, ...)

Procedure in the past:

- Go from SSA (or ℓ_p) to ACF parameters via:

$$\xi = \text{some factor} \cdot \ell_p$$

For the exponential ACF [Mätzler 2002]

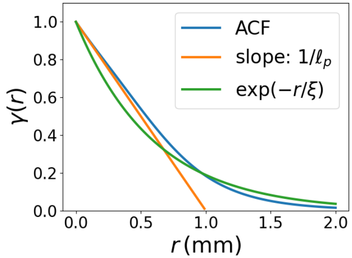
$$d_{SHS} = \text{another factor} \cdot \ell_p$$

For the Sticky Hard Spheres ACF [Brucker 2011, Royer 2017,...]

What if we dont't have ACF measurements?

Snow field measurements:

- Often no μCT $\Rightarrow$ no ACF
- Always SSA estimates (DUFISS, IRIS, IceCube, SMP, InfraSnow, ...)



Procedure in the past:

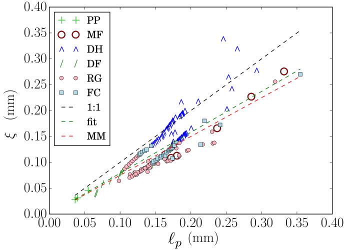
- Go from SSA (or ℓ_p) to ACF parameters via:

$$\xi = \text{some factor} \cdot \ell_p$$

For the exponential ACF [Mätzler 2002]

$$d_{SHS} = \text{another factor} \cdot \ell_p$$

For the Sticky Hard Spheres ACF [Brucker 2011, Royer 2017,...]

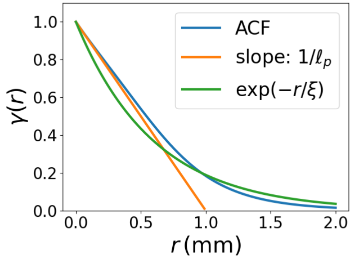


[Krol & Löwe, TC, 2016]

What if we dont't have ACF measurements?

Snow field measurements:

- Often no μCT $\Rightarrow$ no ACF
- Always SSA estimates
  (DUFISS, IRIS, IceCube, SMP, InfraSnow, ...)



Procedure in the past:

- Go from SSA (or ℓ_p) to ACF parameters via:

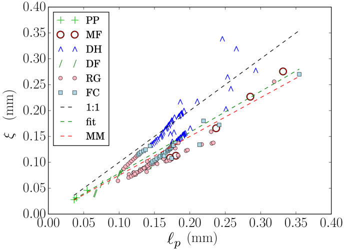
  $$\xi = \text{some factor} \cdot \ell_p$$

  For the exponential ACF [Mätzler 2002]

  $$d_{SHS} = \text{another factor} \cdot \ell_p$$

  For the Sticky Hard Spheres ACF [Brucker 2011, Royer 2017,...]

- Empirical. ACF-model specific.



[Krol & Löwe, TC, 2016]

What we could do instead

Scattering coefficient in IBA

$$\kappa_s \sim k^4 \widetilde{A}(k)$$

$$k \quad : \quad \text{wavenumber}$$

$$\widetilde{A}(k) \quad : \quad \text{Fourier Transform of the ACF}$$

Dimension of $\widetilde{A}(k)$: m^3

What we could do instead

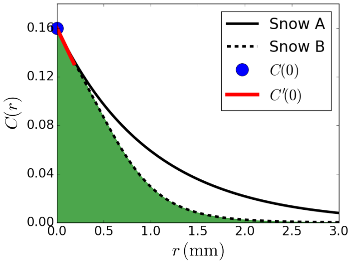
Scattering coefficient in IBA

$$\kappa_s \sim k^4 \widetilde{A}(k)$$

k : wavenumber

$\widetilde{A}(k)$: Fourier Transform of the ACF

Dimension of $\widetilde{A}(k)$: m^3



Suggests definition of microwave grain size:

$$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3} = \left(4\pi \int_0^\infty dr r^2 A(r)\right)^{1/3}$$

[Picard et al, 2022]

What we could do instead

Scattering coefficient in IBA

$$\kappa_s \sim k^4 \widetilde{A}(k)$$

k : wavenumber

$\widetilde{A}(k)$: Fourier Transform of the ACF

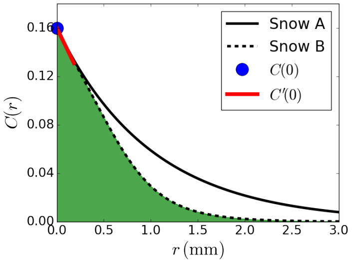
Dimension of $\widetilde{A}(k)$: m^3

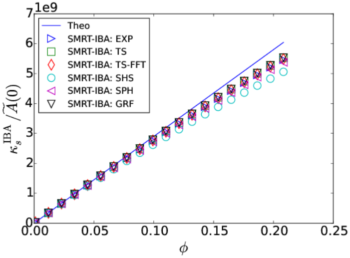
Suggests definition of microwave grain size:

$$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3} = \left(4\pi \int_0^\infty dr r^2 A(r)\right)^{1/3}$$

[Picard et al, 2022]

- Definition independent of any model!





Geometrical interpretation of the microwave grain size

A little algebra reveals:

$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3}$ zero frequency Fourier transform of the ACF

Geometrical interpretation of the microwave grain size

A little algebra reveals:

$$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3} \quad \text{zero frequency Fourier transform of the ACF}$$

$$= \ldots \quad \text{rewritten as the Laplace transform of the ACF}$$

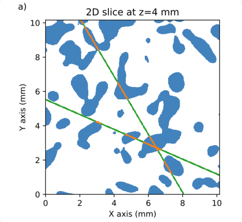
Geometrical interpretation of the microwave grain size

A little algebra reveals:

$$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3}$$ zero frequency Fourier transform of the ACF

$$= \ldots$$ rewritten as the Laplace transform of the ACF

$$= \ldots$$ related to the Chord length distribution (CLD)



Geometrical interpretation of the microwave grain size

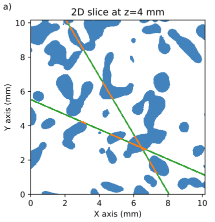
A little algebra reveals:

$$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3}$$ zero frequency Fourier transform of the ACF

$$= \ldots$$ rewritten as the Laplace transform of the ACF

$$= \ldots$$ related to the Chord length distribution (CLD)

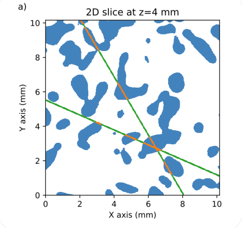
$$= K\ell_{\mathrm{p}}$$ admits a geometrical interpretation



Geometrical interpretation of the microwave grain size

A little algebra reveals:

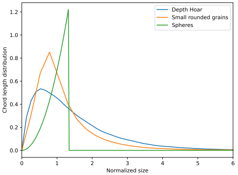
$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3}$	zero frequency Fourier transform of the ACF
$= \dots$	rewritten as the Laplace transform of the ACF
$= \dots$	related to the Chord length distribution (CLD)
$= K\ell_{\mathrm{p}}$	admits a geometrical interpretation



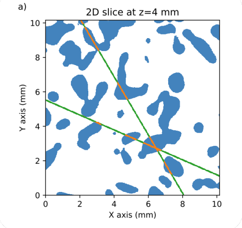
Polydispersity:

$$K = \left(\frac{\mu_4}{24\mu_1^4} - \frac{\mu_2\mu_3}{6\mu_1^5}\phi + \frac{\mu_2^3}{8\mu_1^6}\phi^2\right)^{1/3}(1-\phi)^{-2/3}$$

(ϕ: relative density, μ_i: moments of the CLD, approximation based on [Roberts 1999])



Geometrical interpretation of the microwave grain size



A little algebra reveals:

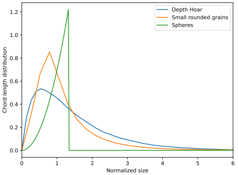
$$\ell_{\mathrm{MW}} := \widetilde{A}(0)^{1/3}$$ zero frequency Fourier transform of the ACF

$$= \ldots$$ rewritten as the Laplace transform of the ACF

$$= \ldots$$ related to the Chord length distribution (CLD)

$$= K\ell_{\mathrm{p}}$$ admits a geometrical interpretation

Polydispersity:



$$K = \left(\frac{\mu_4}{24\mu_1^4} - \frac{\mu_2\mu_3}{6\mu_1^5}\phi + \frac{\mu_2^3}{8\mu_1^6}\phi^2\right)^{1/3} (1-\phi)^{-2/3}$$

(ϕ: relative density, μ_i: moments of the CLD, approximation based on [Roberts 1999])

What we gained:

Geometrical link: Low frequency microwave scattering $\longleftrightarrow$ Optical measurements

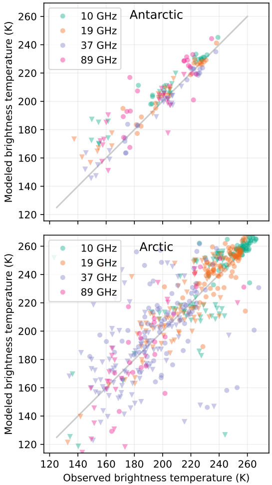
Exploiting the microwave grain size with SMRT

(cf. `smrt.microstructure.unified*`)

From SSA to microwave predictions:

- Inverse: Retrieval of polydispersity
- Forward: Use an educated guess for K

Emission: SMRT vs Measurements



[Picard et al, 2022]

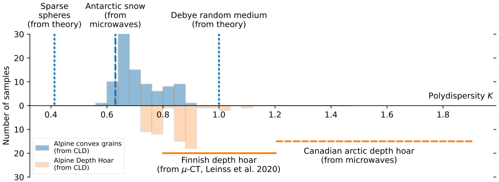
Exploiting the microwave grain size with SMRT

(cf. `smrt.microstructure.unified*`)

From SSA to microwave predictions:

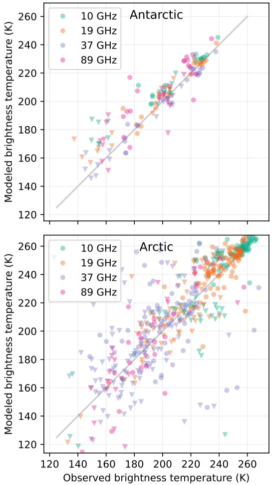
- Inverse: Retrieval of polydispersity
- Forward: Use an educated guess for K

Polydispersity distribution



[Picard et al, 2022]

Emission: SMRT vs Measurements



[Picard et al, 2022]

Summary

The two-point (or autocorrelation) function of snow:

- Dictates microwave scattering
- Defines microwave grain size and reveals difference to optical grain size

Summary

The two-point (or autocorrelation) function of snow:

- Dictates microwave scattering
- Defines microwave grain size and reveals difference to optical grain size

Microstructure in SMRT:

- Represented by parametric ACF forms
- An SMRT snowpack can comprise layers with different ACFs
- New ACF models can be easily added by implementing $C(r)/\widetilde{C}(k)$
- Not explored yet: Using measured ACF data directly (need for regularization)

Thank you for your attention.