SMRT Microstructure

Henning Löwe

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

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Outline

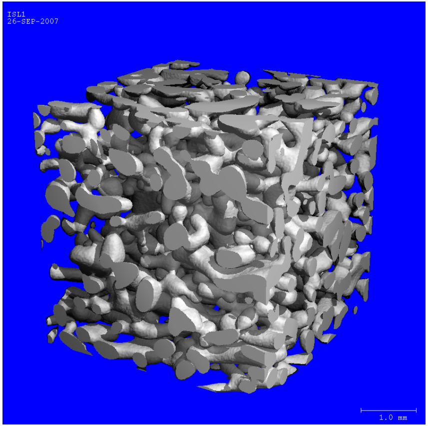
Motivation

Background on correlation functions

Microstructure implementation in SMRT

Microstructure in SMRT

Snow microstructure as nowadays seen by X-ray tomography:



- A primary goal of SMRT: Faithful representation of microstructure

Recap from EM lecture: Where microstructure matters

IBA phase function:

$$p\,(\vartheta, \varphi)_{\text{1-2 frame}} = f_2(1 - f_2)(\epsilon_2 - \epsilon_1)^2\; Y^2(\epsilon_1, \epsilon_2)\; k_0^4\; M(|\mathbf{k}_d|)\, \sin^2\chi \tag{1}$$

Microstructure term:

$$M(|\mathbf{k_d}|) = \frac{1}{4\pi} \frac{\widetilde{C}(|\mathbf{k}_d|)}{f_2(1 - f_2)}. \tag{2}$$

is related to the Fourier transform $\widetilde{C}(|\mathbf{k}_d|)$ of the two-point correlation function or auto-correlation function (ACF).

$\rightarrow$ Need to understand this term.

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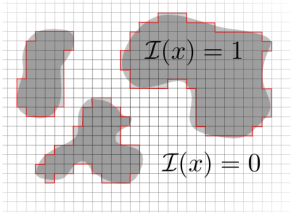
Definition and properties of the ACF

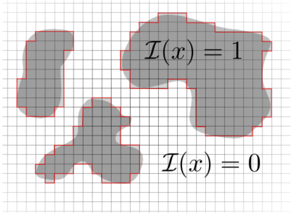
Indicator function of the ice phase:



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

- A binary image (μCT, thin section) is a discrete version of it

Definition and properties of the ACF



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Auto-correlation function (ACF):

$$\begin{aligned} C(\mathbf{r}) &= \overline{\left(\mathcal{I}(\mathbf{x}) - f_2\right)\left(\mathcal{I}(\mathbf{x}+\mathbf{r}) - f_2\right)} \\ &= \overline{\left(\mathcal{I}(\mathbf{x})\mathcal{I}(\mathbf{x}+\mathbf{r}) - f_2^2\right)} \end{aligned}$$

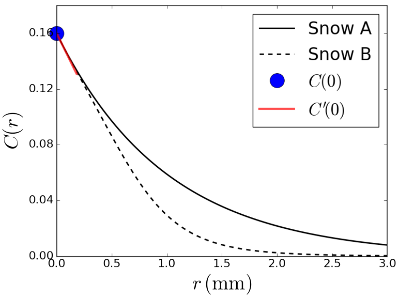
- Fluctuations around the mean (volume fraction f_2)
- Spatial (two-point) statistics of the ice-air assembly

Why is an ACF more than SSA and density?

Can be seen from special ACF values:

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

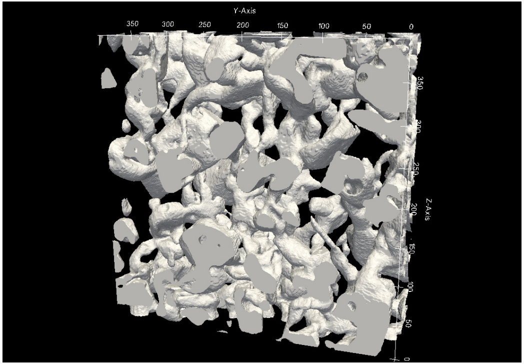
(schematic)

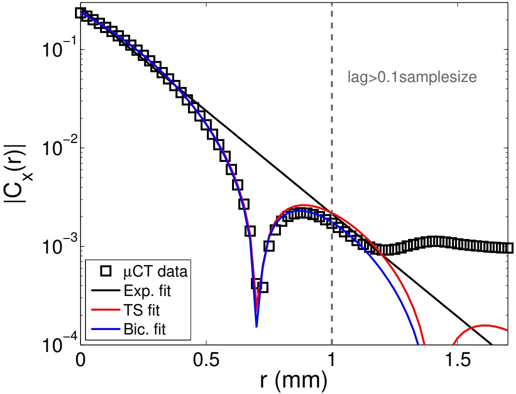


- SSA and density characterize only the behavior of $C(r \approx 0)$: small scale correlations
- Microstructures with the same density and the same SSA can have completely different "correlation tails"
- Single length scale models (like exponential) seem to be insufficient

A real example to demonstrate this

- Apparently “simple snow” does not have “simple correlations”:



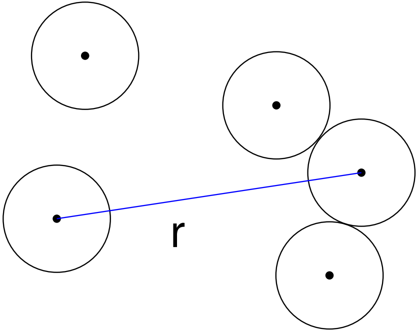


- We don't understand yet why, but SMRT shouldn't suffer from that
- More on that $\rightarrow$ practical

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

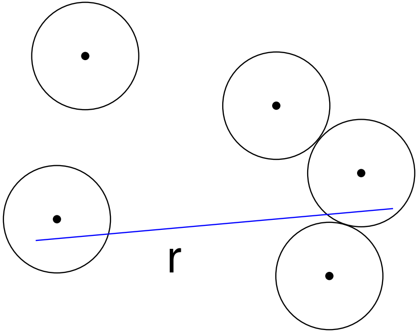
Commonly formulated in different types of correlation functions:

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

Computing the ACF from pair correlations:

Exact result for arbitrary (hard) sphere packings: (Stell & Torquato, 1982)

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

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

Or in Fourier space

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

- $P(\boldsymbol{k})$: form factor, $S(\boldsymbol{k})$: structure factor (small angle scattering lingo)

This link allows to...

- map μCT images onto arbitrary hard-sphere packings
- implement DMRT's sticky hard spheres in IBA
- compare EM formulations from DMRT and IBA

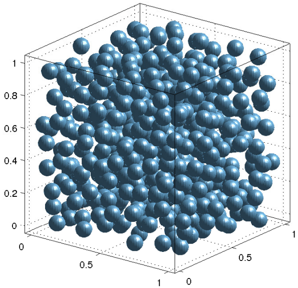
(Löwe & Picard, 2015)

A good point to demystify "sticky hard spheres"

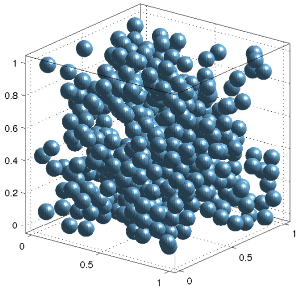
Model for a molecular fluid (Baxter, 1967)

- Determined by volume fraction f_2, diameter d, and stickiness τ

Example realizations: (identical $f_2, d \to$ same SSA!!)



$\tau = 10.0$



$\tau = 0.11$

(Code acknowledgements: L. Tsang)

Main effect of stickiness τ:

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

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Considered models in SMRT and reasons for them ($C(r) = C(0)A(r)$)

Exponential: Used by MEMLS

$$A_{\mathrm{ex}}(r) = \exp(-r/l_{\mathrm{ex}}) \tag{3}$$

Sticky hard spheres: Used by DMRT-ML, DMRT-QMS

$$\text{(defined in Fourier space)} \tag{4}$$

Independent sphere: A classic ("spherical acf model"), sparse medium model

$$A_{\mathrm{sph}}(r) = \left[1 - 3\left(r/d_{\mathrm{sph}}\right)/2) + \left(r/d_{\mathrm{sph}}\right)^3/2\right] H(d_{\mathrm{sph}} - r) \,, \tag{5}$$

Teubner–Strey: Google "scattering peak" and "bicontinuous"...

$$A_{\mathrm{TS}}(r) = \exp(-r/\xi_{\mathrm{TS}}) \frac{\sin(2\pi r/d_{\mathrm{TS}})}{(2\pi r/d_{\mathrm{TS}})} \,, \tag{6}$$

(Level cut) Gaussian random fields: Most powerful in the long term

$$C_{\mathrm{grf}}(r) = \frac{1}{2\pi} \int_0^{C_\psi(r)} dt \frac{1}{\sqrt{1-t^2}} \exp\left[-\frac{\beta^2}{1+t}\right] \tag{7}$$

Microstructure implementation in SMRT

Abstract base class:

```
class Autocorrelation (autocorrelation.py)
```

- Handles common functionality: Numerical Fourier transforms

Derived microstructure classes:

```
class Exponential (exponential.py)
class StickyHardSpheres (sticky_hard_spheres.py)
class IndependentSphere (independent_sphere.py)
class GaussianRandomField (gaussian_random_field.py)
class TeubnerStrey (teubner_strey.py)
class MeasuredAutocorrelation (measured_autocorrelation.py)
```

- Hold microstructure parameters
- Compute analytical autocorrelation functions (if available)
- Must implement either $C(r)$ or $\widetilde{C}(k)$.
- Here you can easily add your ultimate ACF model

Practically: How is $C(r)$ obtained from images?

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

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

- $C(\boldsymbol{r})$ is computed from 2D/3D images via FFT and parameters are obtained by fitting ($\rightarrow$ practical)
- Hint: FFT is a python one-liner $\mathcal{F}(g) \rightarrow$ `fftpack.fftn(g)`

What about microstructural anisotropy?

$C(\boldsymbol{r})$ of an anisotropic 3D image is a anisotropic 3D ACF

- SMRT microstructure only deals with 1D functions $C(r)$ (isotropy)
- Different ways to create an isotropoic $C(r)$

But the IBA phase function requires a 3D Fourier transform anyway? Yes:

- 3D Fourier transforms of isotropic $C(r)$ can be written as 1D Bessel transforms and computed via a discrete 1D sine transform:

$$\widetilde{C}(k) = 4\pi \int_0^\infty dr\, r^2 C(r)\, j_0(kr) \quad (8)$$

$$= 4\pi/k\, \Delta r \underbrace{\sum_{l=0}^{N-1} \sin(kr_m) \left[\frac{C(r_m)}{r_m}\right]}_{\frac{1}{2}\mathrm{DST}(k)} \quad (9)$$

- Thats how its done in SMRT `autocorrelation` class

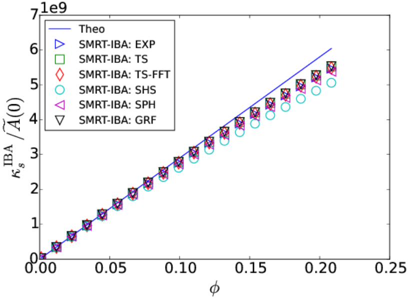
All SMRT μ-models at a glance: Limiting case of the scattering coefficient

Asymptotic expansion of IBA:

The IBA Scattering coefficient for *low density*, *low frequency* has a microstructure dependent limiting behavior:

$$\kappa_{\mathrm{s}}^{\mathrm{IBA}} = \left[\frac{2}{3} k_0^4 \frac{1}{4\pi}(\epsilon_2 - \epsilon_1)^2 \left|\frac{3\epsilon_1}{2\epsilon_1 + \epsilon_2}\right|^2\right] f_2\, \widetilde{A}(0)$$

Comparison with SMRT:



Summary

Microstructure in SMRT:

- Employs ACF of snow as required by IBA
- Envisages a library concept, similar to small angle scattering software
- An SMRT snowpack can comprise SMRT layers with different ACFs
- New ACF models can be added by implementing another forms for $C(r)/\widetilde{C}(k)$
- Foreseen but not explored yet: Using measured ACF data directly
- Ongoing research: Details of parameter retrieval by fitting 3D images

Thank you for your attention.