Spatial statistical analysis of micro-structures of nano silica particle gels

PASI 2014

Henrike Häbel

Aila Särkkä, Mats Rudemo and Matias Nordin*

Mathematical Sciences, Chalmers University of Technology
*German Cancer Research Center

Content

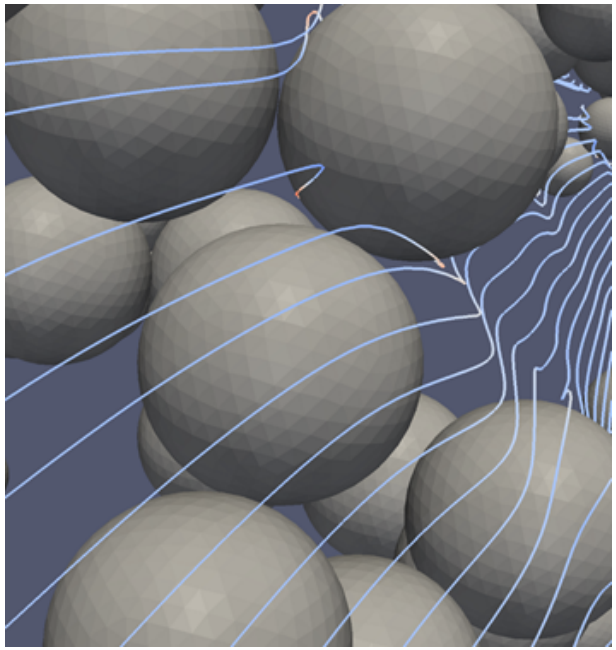
Nano silica particle gels
- RLCA process

Spatial Statistical Analysis
- Spatial summary statistics
- RLCA parameter estimation

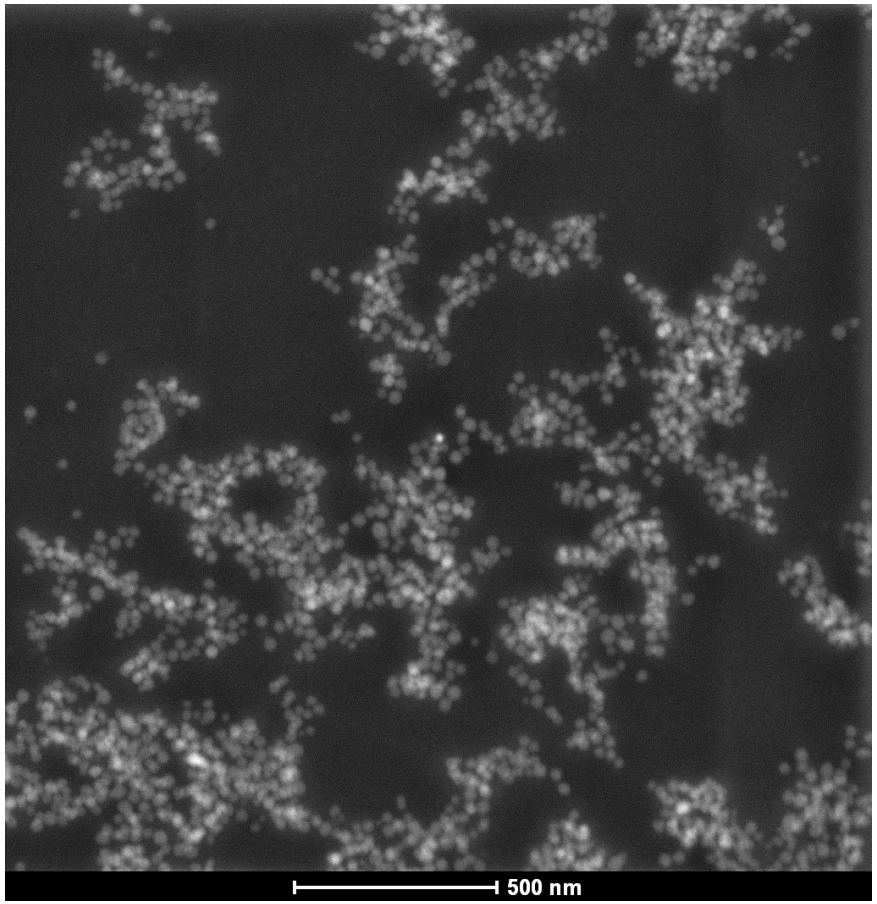
Conclusion and Outlook

Motivation: Mass transport

- Mass transport:
  Diffusion and flow
- Nano silica particle gels as
  test bed for mass transport

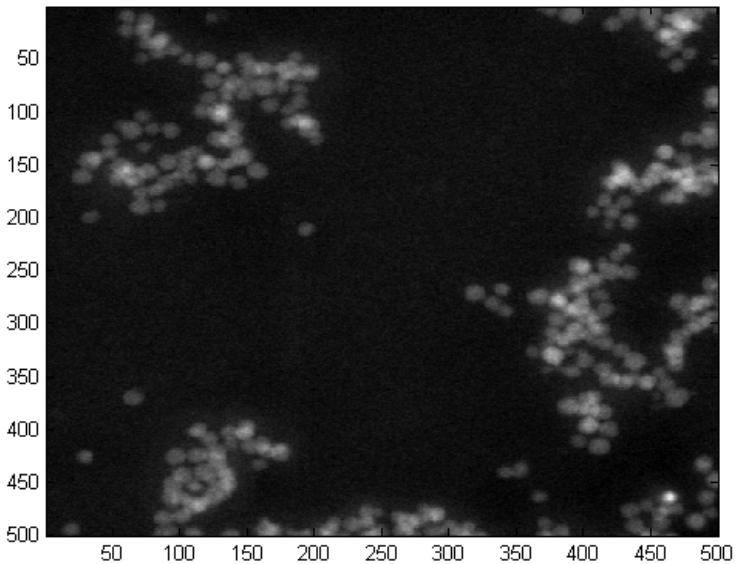


Nano silica particle gels

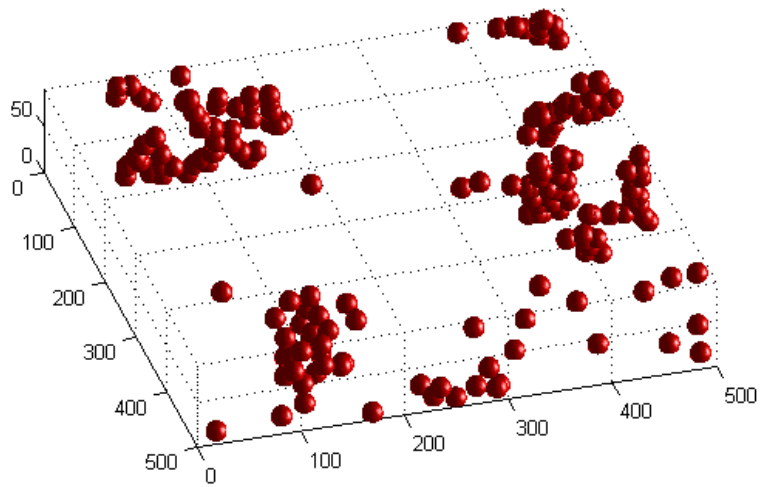


STEM micrograph of 90nm thick silica particle (20nm) gel

Goal: 3D reconstruction of micro-structure

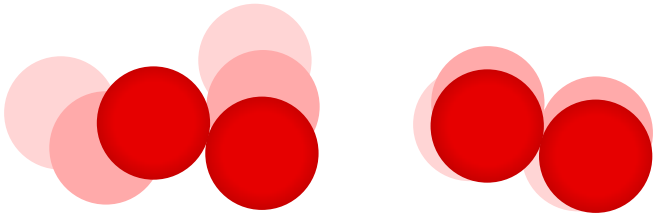


500x500 nm section of micrograph



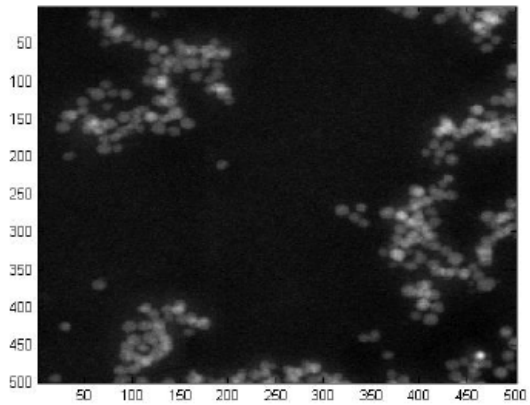
3D reconstruction based on mass thickness estimation

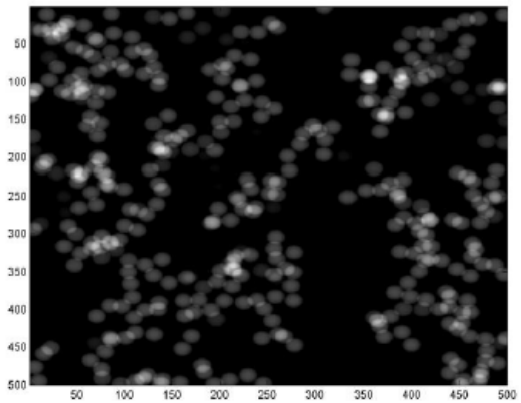
RLCA process

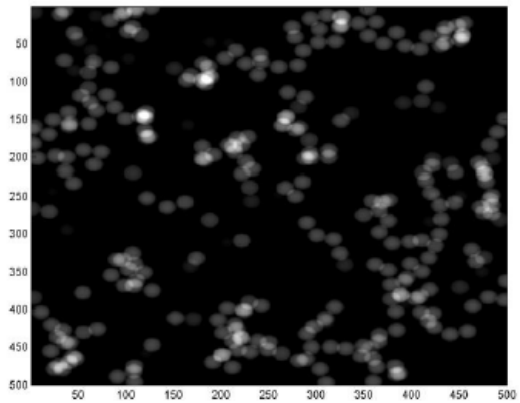


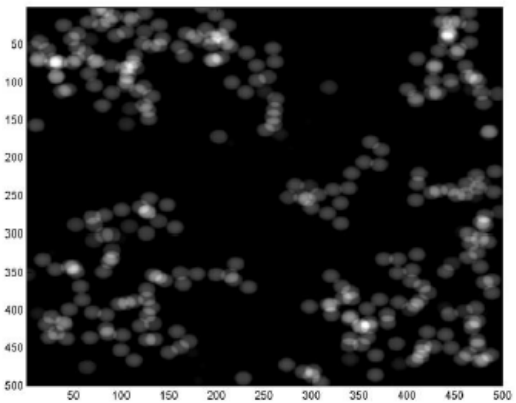
- Reaction limited cluster aggregation (RLCA)
- Particle diffusion according to Brownian motion
- Sticking probability: $P_{stick} \in [0, 1]$
- The larger the cluster the smaller the diffusion coefficient

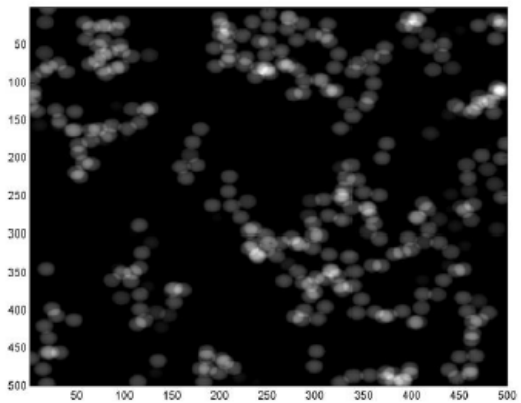
Sticking probability: $P_{stick} \in [0, 1]$

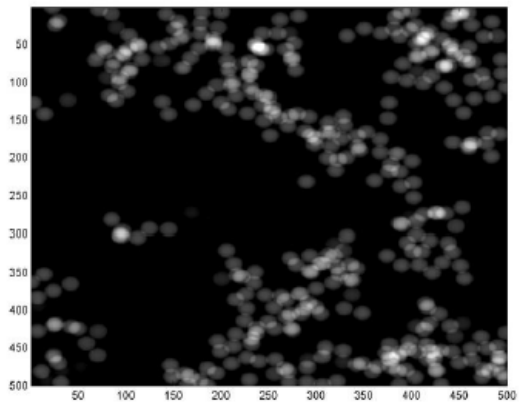

data


p = 1


p = 0.1


p = 0.01


p = 0.001


p = 0.0001

Spatial summary statistics

Task: Find suitable spatial summary statistics to characterize different particle configurations

Three first candidates:

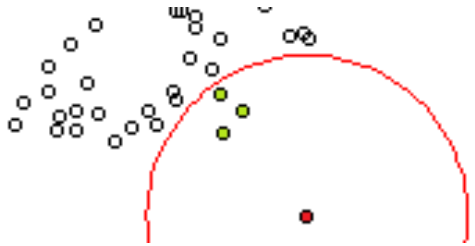
- Pair-correlation function
- Empty space function
- Cluster function

Pair-correlation function

Ripley's K-function

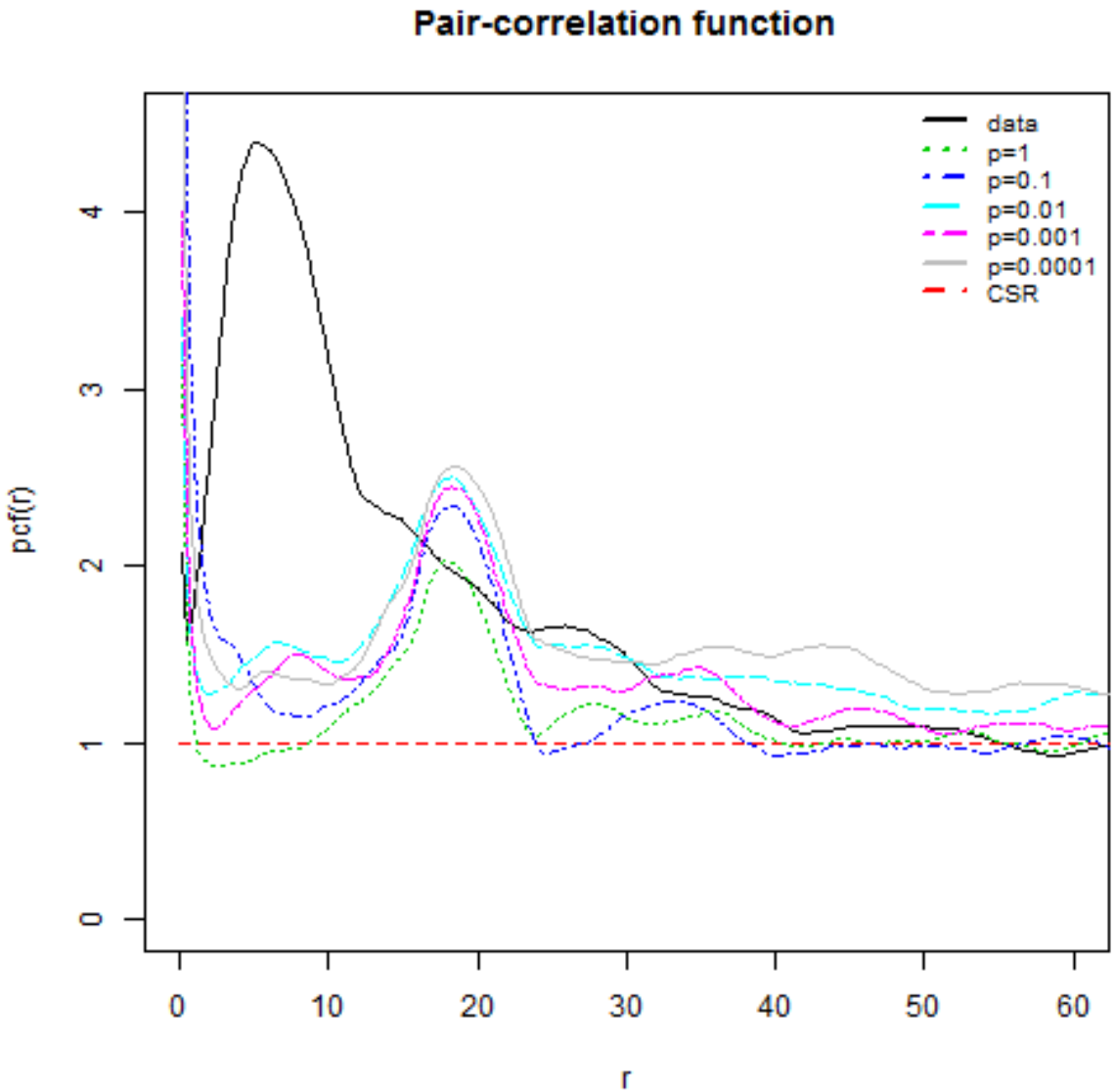
$$K(r) = \lambda^{-1}\mathbb{E}_o(\Phi(b(o,r)) \setminus \{o\}) \quad r \geq 0$$

with expectation w.r.t. Palm distribution given a point exists in o



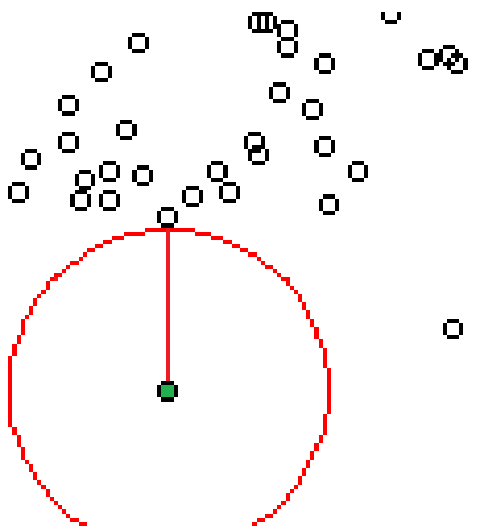
Pair-correlation function

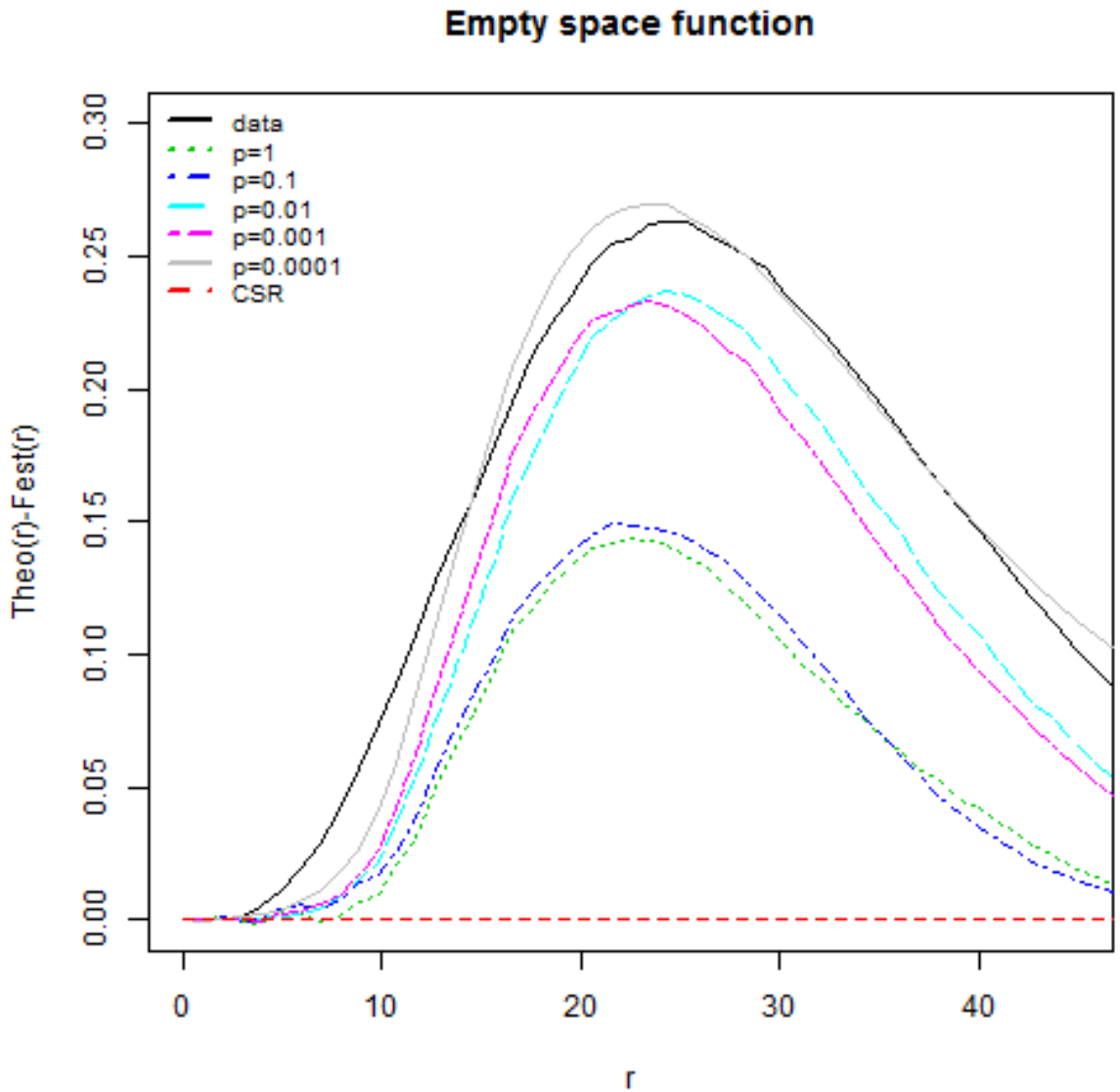
$$\rho(r) = \frac{\mathrm{d}\mathbb{E}(\Phi(b(o,r)))/\mathrm{d}r}{\lambda d\nu_d(b(o,1))r^{d-1}} \quad r \geq 0$$


Pair-correlation function
data
p=1
p=0.1
p=0.01
p=0.001
p=0.0001
CSR
pcf(r)
0
1
2
3
4
0
10
20
30
40
50
60
r

Empty space function

$$
\begin{aligned}
F(r) &= \mathbb{P}(\inf\{\|o - x\| : x \in \Phi\} \leq r) \\
&= 1 - \mathbb{P}(\Phi(b(o, r)) = 0) \qquad\qquad r \geq 0
\end{aligned}
$$

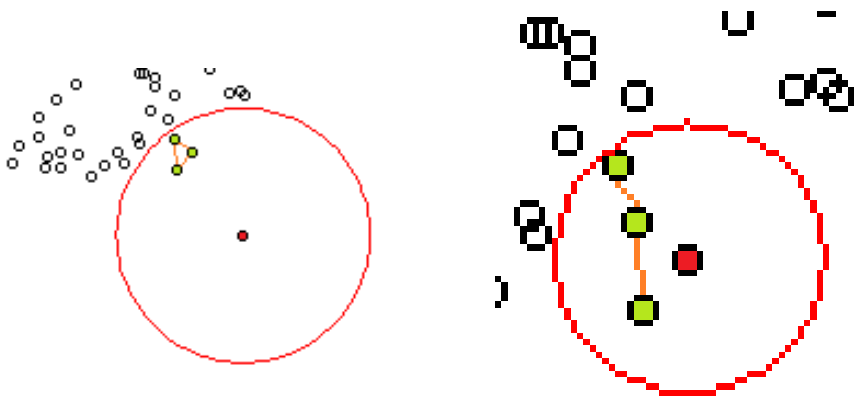


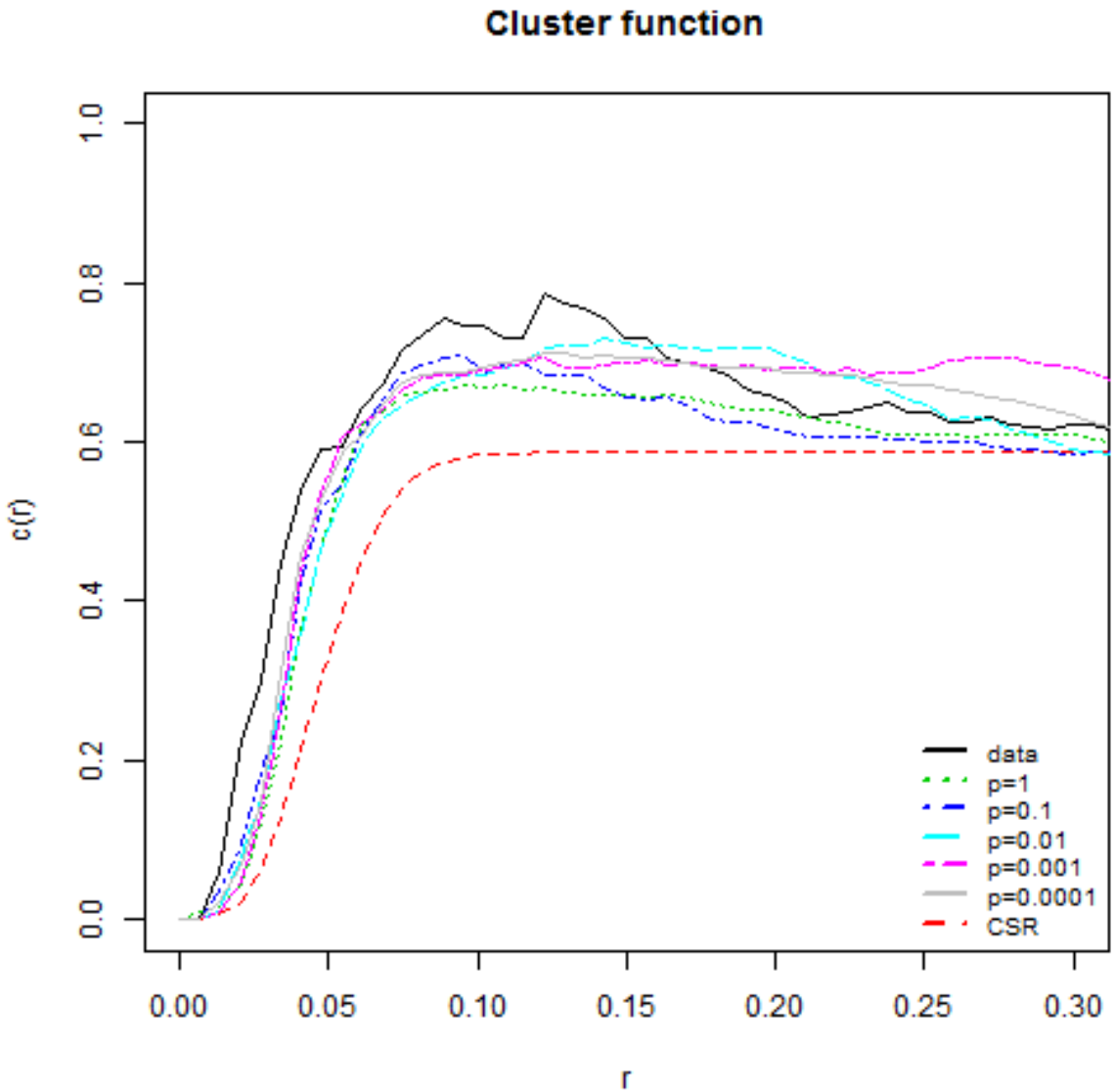

Empty space function
data
p=1
p=0.1
p=0.01
p=0.001
p=0.0001
CSR
Theo(r)-Fest(r)
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
10
20
30
40
r

Cluster function

$$c(r) = \frac{1}{n} \sum_i \frac{\sum_{j,k \in \partial(i)} \mathbb{I}(\|X_j - X_k\| \leq r)}{\binom{|\partial(i)|}{2}} \quad r \geq 0$$

for n points and neighborhood ∂ defined via $\|\cdot\| \leq r$




Cluster function
c(r)
r
0.0
0.2
0.4
0.6
0.8
1.0
0.00
0.05
0.10
0.15
0.20
0.25
0.30
data
p=1
p=0.1
p=0.01
p=0.001
p=0.0001
CSR

Sticking probability estimation

LS-type approach:

for i in grid

1. Generate RLCA reconstruction with $P_{stick} = p_i$
2. Compare to real data by calculating

$$S_i = \omega_1 S_1 + \ldots \omega_k S_k$$

for features $S_1, \ldots, S_k$ describing the spatial structure of the particles

end

Find $i_{min} = argmin_i(S_i)$ and select $P_{stick} = p_{i_{min}}$

Conclusions and Outlook

Goal: Estimate RLCA sticking probability using spatial statistics

- Current step: Finding spatial summary statistics
  - Normalize real and simulated data
  - k^{th} nearest neighbors
  - Develop gray scale based summary statistics

- Next step:
  - Validation of concept in a simulation study
  - Analyze 3D data

References

Moncho-Jordá, A., Odriozola, G., Martínez-López, F., Schmitt, A., Hidalgo-Álvarez, R. (2001). The DLCA-RLCA transition arising in 2D-aggregation: simulations and mean field theory. *The European Physical Journal E,* 5 (pp. 672-683).

Nordin, M., Abrahamsson, C., Blomqvist, C.H., Häbel, H., Röding, M., Olsson, E., Nydén, M., Rudemo, M.(2014). Estimation of mass thickness response of embedded aggregated silica nanospheres from high angle annular dark-field scanning transmission electron micrographs. *Journal of Microscopy,* 253 (2) (pp. 166-170).

Rajala, T. (2010). Spatial clustering and graph based statistical features. *JYU preprints*.

Redenbach, C., Särkkä, A. (2013). Parameter estimation for growth interaction process using spatio-temporal information. *Computational Statistics and Data Analysis,* 57 (pp. 471-480).

Stoyan, D., Kendall, W.S., Mecke, J. (1995). *Stochastic Geometry and its Applications*. Chichester: John Wiley & Sons.

Thank you very much for your attention!