An Algorithm for Evaluating Fractal Parameters of a Single Soot Aggregate

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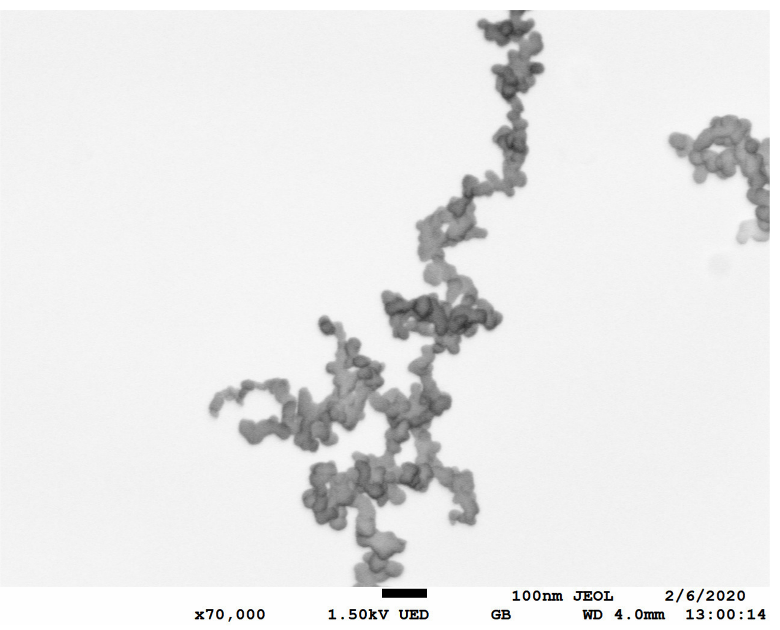
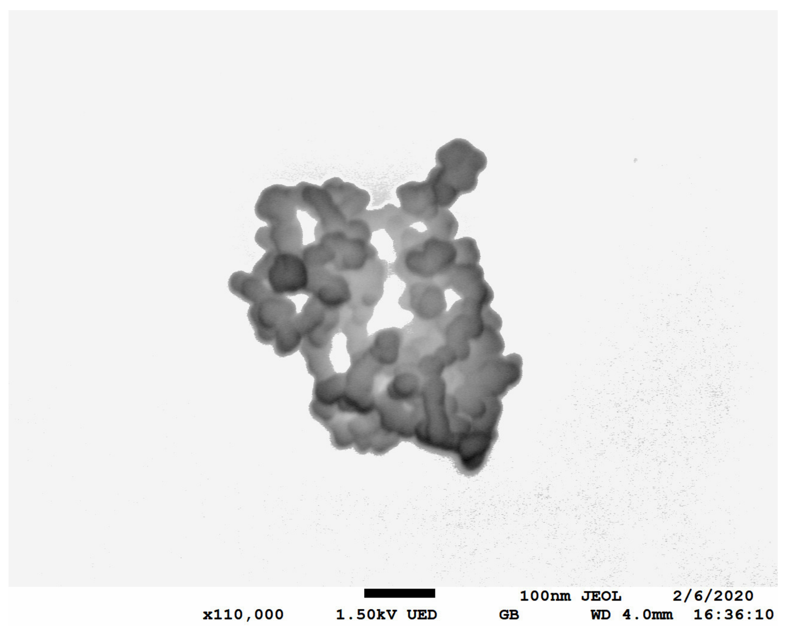
Introduction

- Soot particles are aggregates of carbon spherules
- Their morphology is often described using fractal law
- Soot particles restructure as they age in the atmosphere and the degree of aging is usually quantified using fractal dimension
- We are developing a model for soot restructuring and we need to be able to determine the fractal parameters at any step in the simulation



Lacey aggregate



Compacted aggregate

Background

Fractal scaling law:

$$N = k_0 \left(\frac{R_g}{a}\right)^{D_f}$$

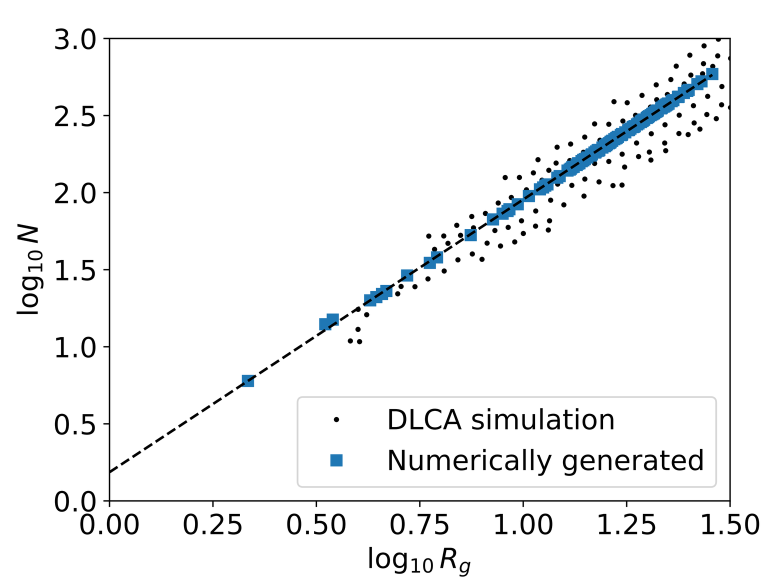
where
N is the number of primary particles
k_0 is the pre-exponential factor
R_g is the radius of gyration of the aggregate
a is the size of a primary particle
D_f is the fractal dimension

Center of mass:

$$\mathbf{r}_0 = \frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i$$

Radius of gyration:

$$R_g^2 = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}_i - \mathbf{r}_0)^2$$



Linear regression on a distribution of numerically generated particles and data from a DLCA simulation [2]

Problem: there are two unknowns, but only one aggregate

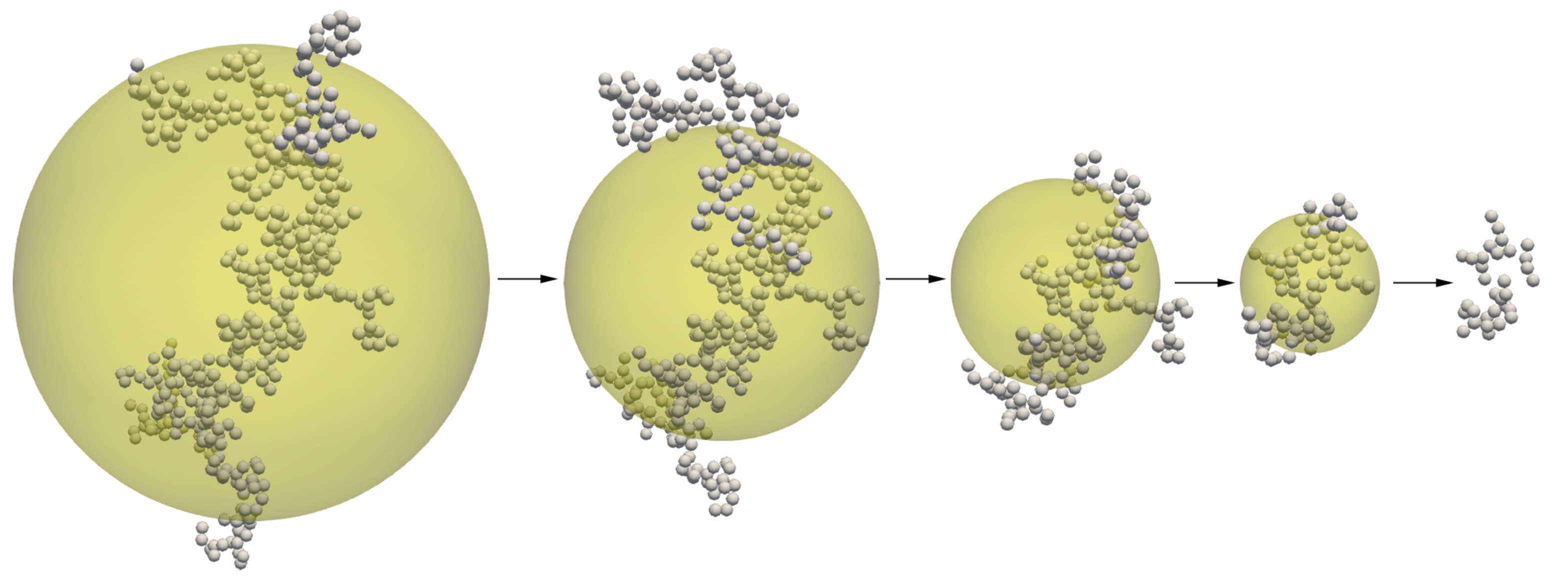
Previous work: Adachi et al. [1] used a voxel-based approach to extract D_f from TEM tomograms

Hypothesis: we can extract sub-aggregates of different sizes and determine the fractal parameters that way

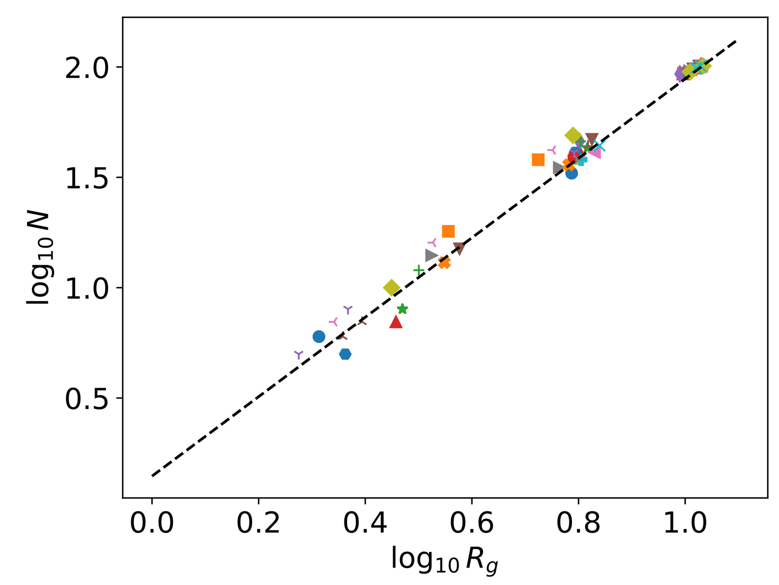
Methodology

1. Aggregates of known (D_f, k_0) were generated with a CCA algorithm
2. The algorithm was applied and results were compared to prescribed parameters
3. Aggregate cut off sizes were adjusted to maximize the accuracy

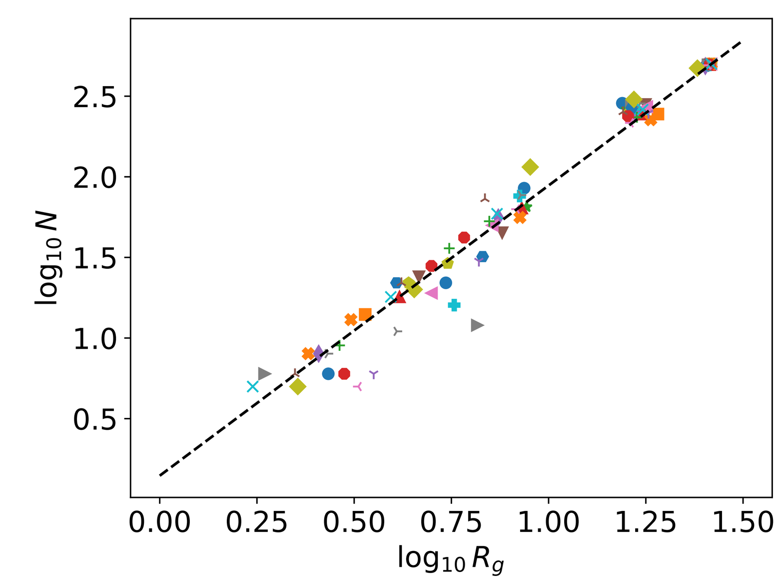
Algorithm



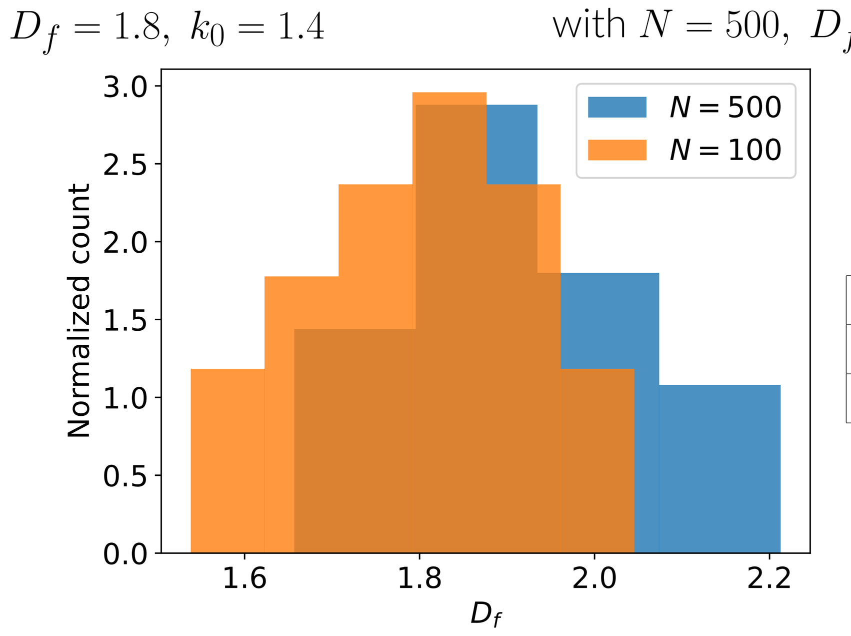
Results - random aggregates



Sub-aggregates extracted from aggregates with $N = 100,\ D_f = 1.8,\ k_0 = 1.4$



Sub-aggregates extracted from aggregates with $N = 500,\ D_f = 1.8,\ k_0 = 1.4$

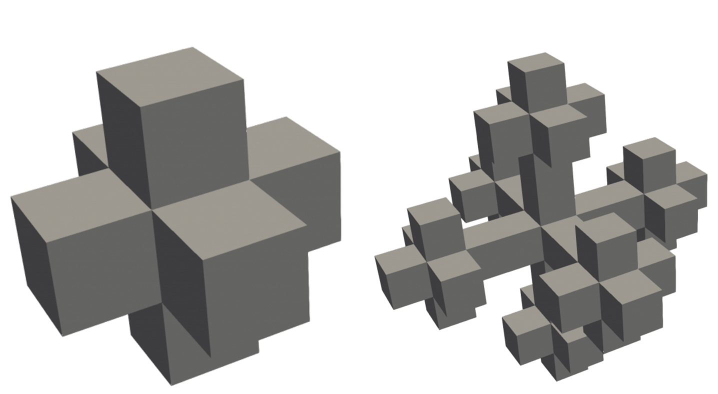


N	100	500
mean	1.80	1.89
stdev	0.13	0.16

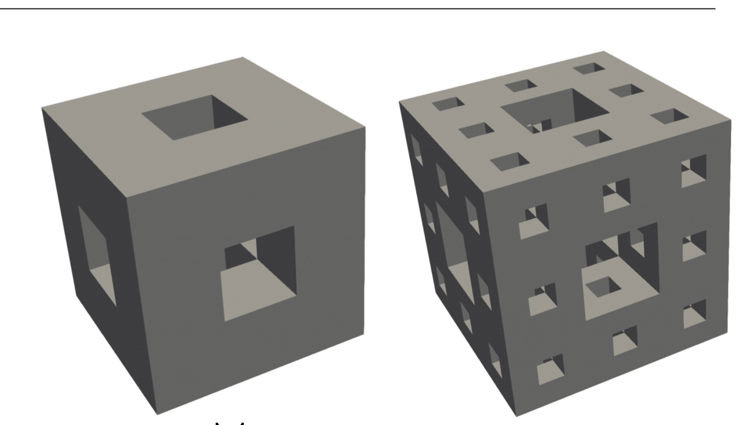
Accuracy for aggregates of different sizes

- The algorithm does not extract fractal parameters exactly, but provides reasonable estimates
- Accuracy is affected by cutoff sizes

Deterministic fractals

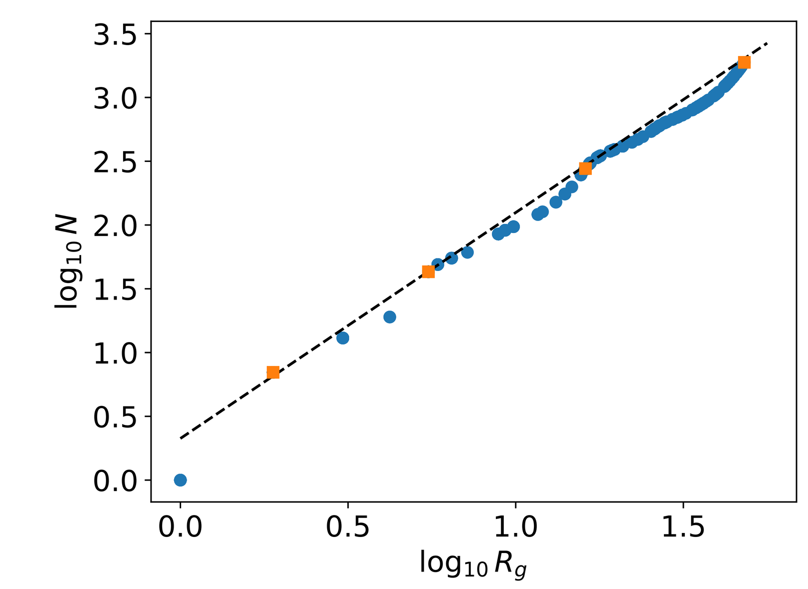


Vicsek fractal
$D_f = \log_3 7 \approx 1.771$



Menger sponge
$D_f = \log_2 4 = 2$

Results - deterministic aggregates



Sub-aggregates extracted from a Vicsek fractal

- The step between sphere sizes affects the results
- Even deterministic aggregates may produce incorrect fractal parameters if wrong step is used
- The step is an intrinsic parameter of the fractal
- For random fractals the optimal step needs to be determined empirically

Conclusion

- While the algorithm may not be able to retrieve the exact values of fractal parameters, it can possibly still be used to track the evolution of a single aggregate
- The algorithm works on aggregates small enough to be representative of typical soot particles

Future work

- Test the algorithm on aggregates with a higher D_f (more compact)
- Apply the algorithm to a restructuring aggregate

Acknowledgment

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E-copy of the poster

Bibliography

(1) Adachi, K.; Chung, S. H.; Friedrich, H.; Buseck, P. R. *Journal of Geophysical Research: Atmospheres* **2007**, *112*.

(2) Heinson, W. R.; Liu, P.; Chakrabarty, R. K. *Aerosol Science and Technology* **2017**, *51*, 12–19.