Retrieval of the fractal parameters of individual soot aggregates

Egor Demidov*[1], Laurence Lu[2], Divjyot Singh[3], Alexei Khalizov[4]

[1]Chemical and Materials Engineering Department, NJIT
[2]Bergen County Technical High School, Teterboro, NJ; now at UC Berkeley
[3]Department of Physics, NJIT; now at Los Alamos National Laboratory, DOE
[4]Chemistry and Environmental Science Department, NJIT

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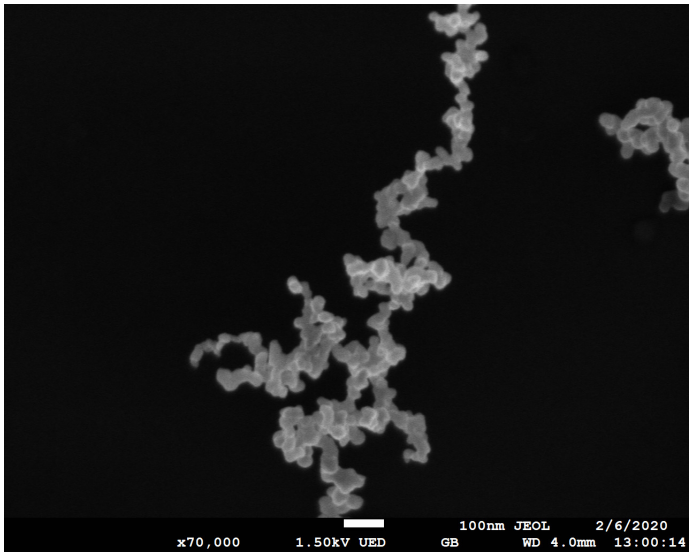
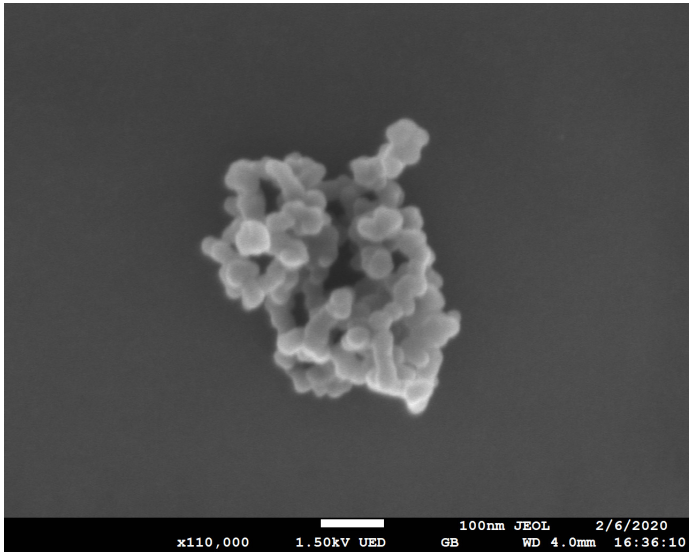
Complex morphology of soot particles

- Carbon soot is released into the atmosphere upon incomplete combustion of fossil fuels
- Soot affects the climate through scattering and absorption of sunlight
- Soot aggregates restructure as they acquire coatings in the atmosphere
- Morphology of aggregates affects their scattering and absorption properties





Characterization of soot morphology

- Aggregate morphology is characterized using fractal law, where N is the number of primaries, R_g is the radius of gyration, k_0 is pre-factor, and D_f is fractal dimension
- D_f directly relates to degree of restructuring of an aggregate
- There are several popular methods for calculation of fractal parameters of aggregates, including box count and ensemble

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

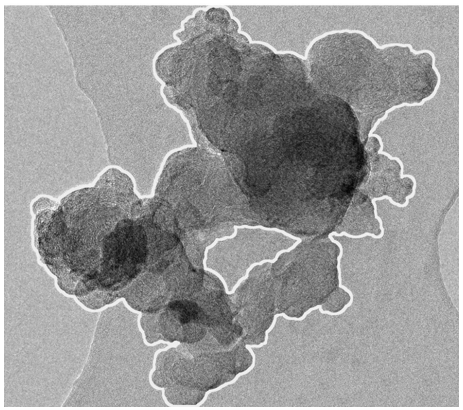
Key takeaway

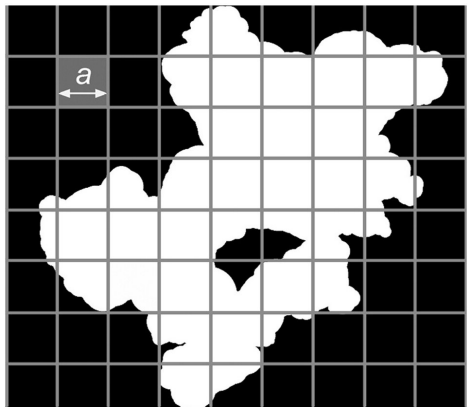
There are two unknown variables k_0 and D_f, which makes the calculation non-trivial

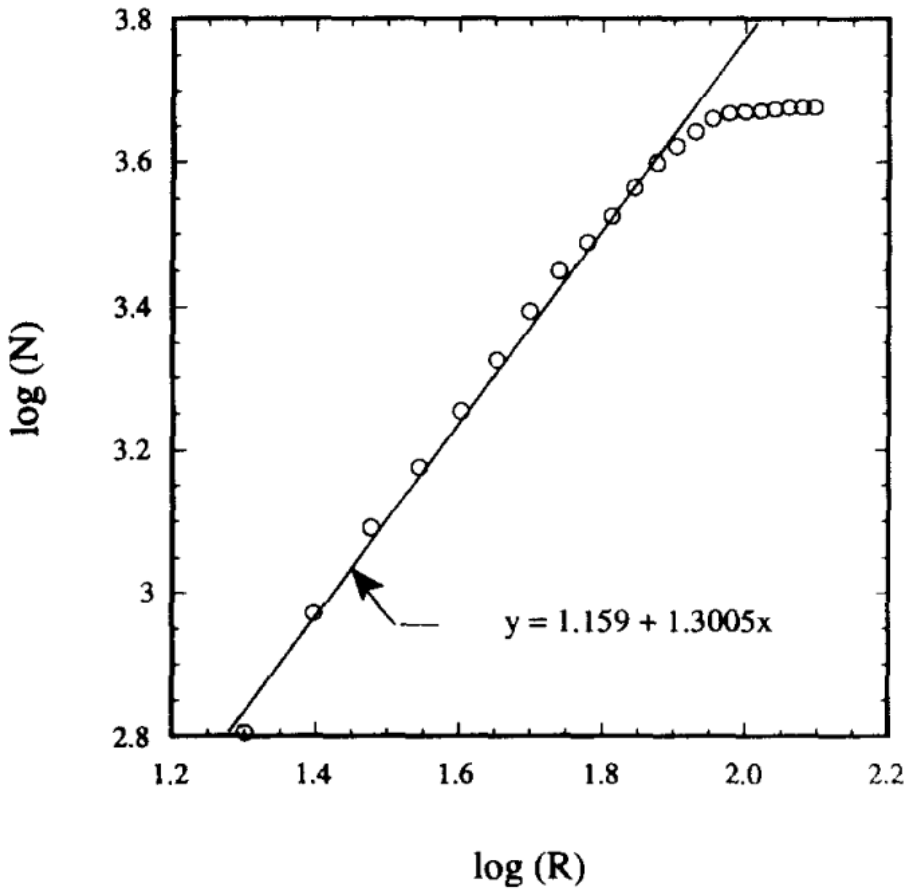
Box count method

Is used for fractal analysis of soot images (2D). It involves covering the aggregate's projection with grids of increasing caliber (box size a)

$$C = k_0 a^{-D_f}$$







Key takeaway

Box count method is not representative of real 3D aggregates

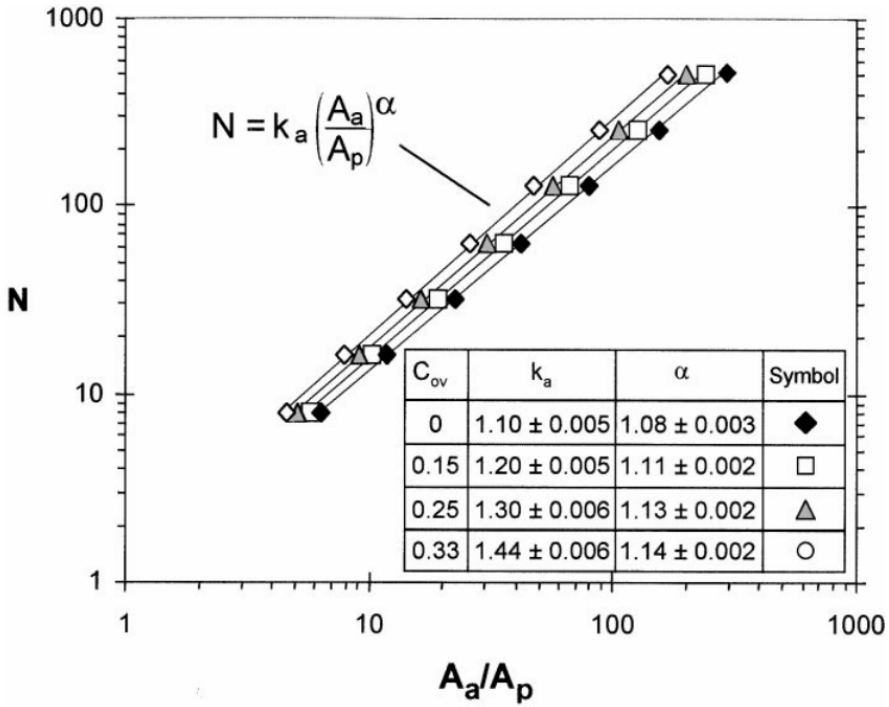
Ensemble method

Requires identifying the projected area of a monomer and the projected area of the aggregate

$$N = k_a \left(\frac{A_a}{A_p} \right)^{\alpha}$$

$$\frac{L_{max}}{2R_g} = 1.50$$

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

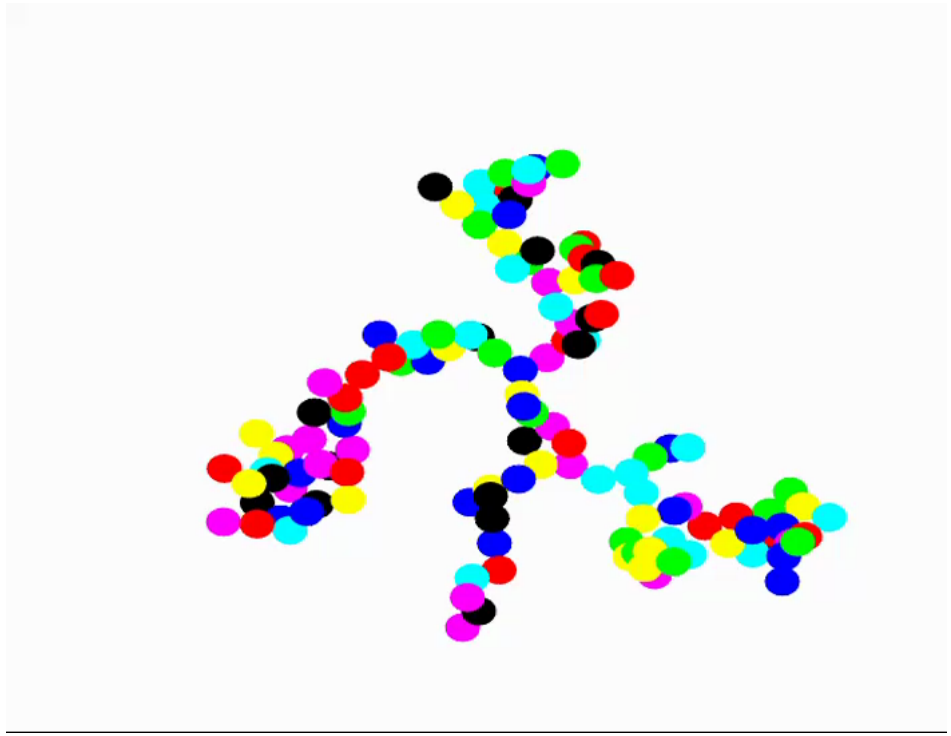


Key takeaway

Ensemble method cannot be used on a single aggregate

A model for soot restructuring

- Our group has been working on modeling the restructuring process of soot
- To track how the system evolves over time, it is necessary to calculate D_f and k_0 of the aggregate at any point
- Both D_f and k_0 change as the aggregate collapses



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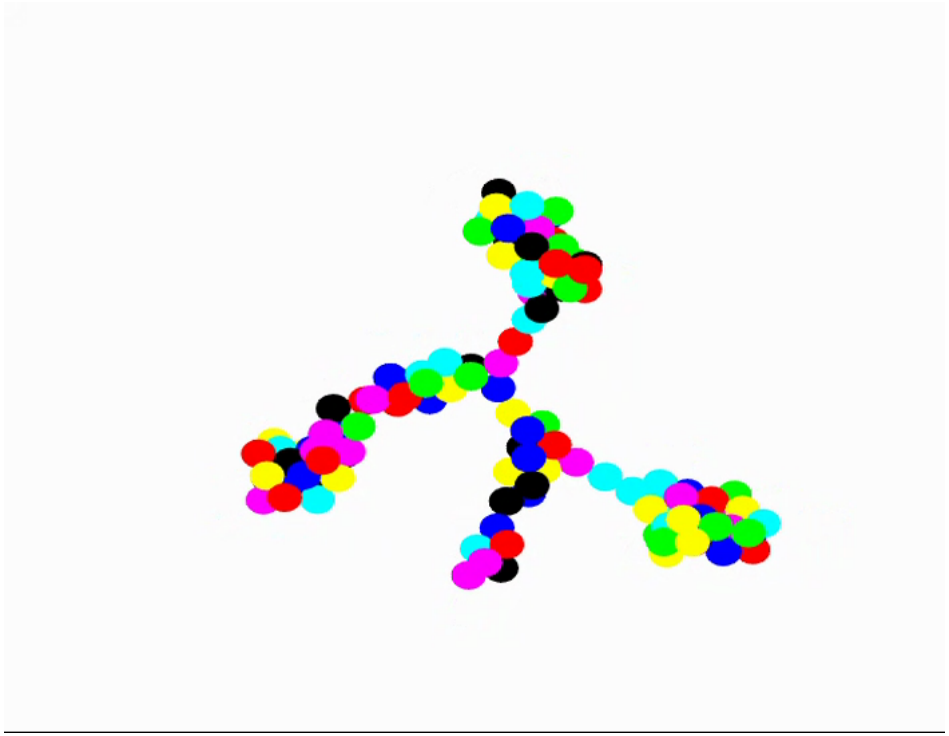

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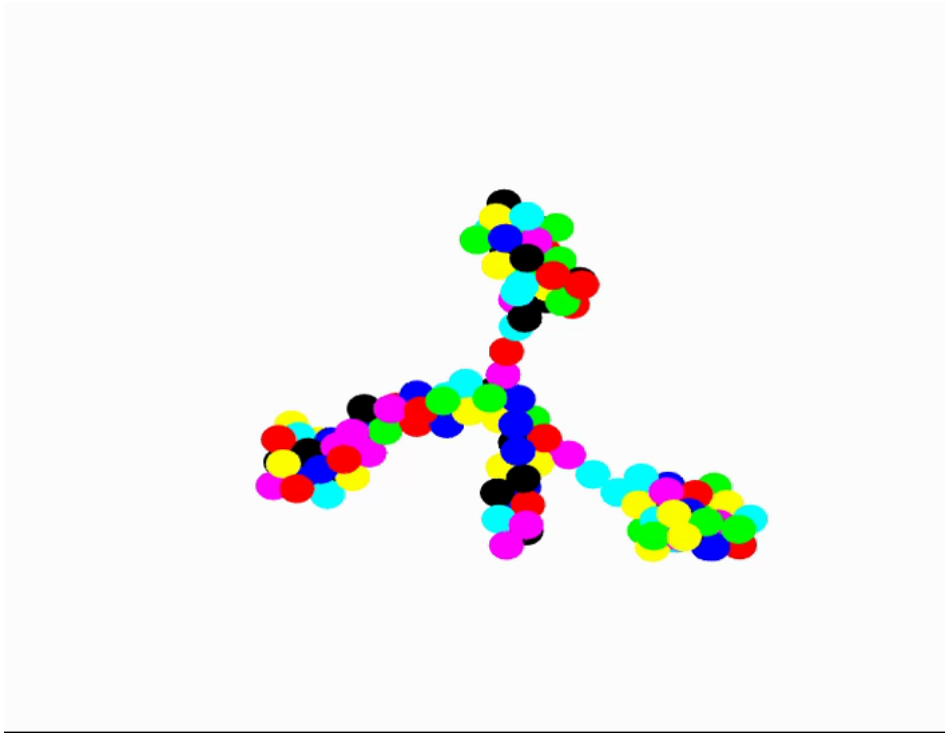

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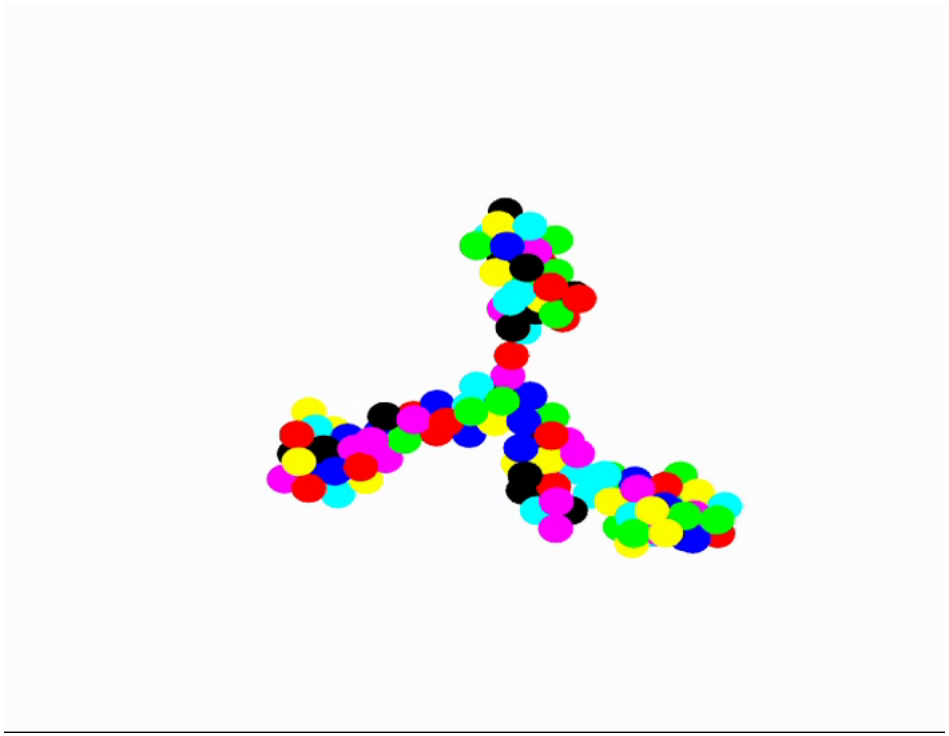

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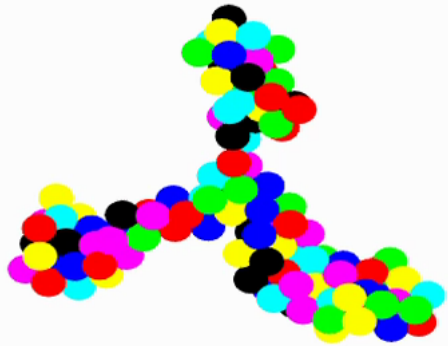

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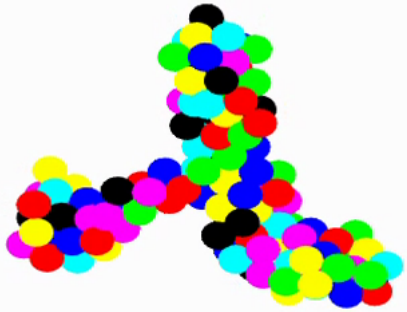

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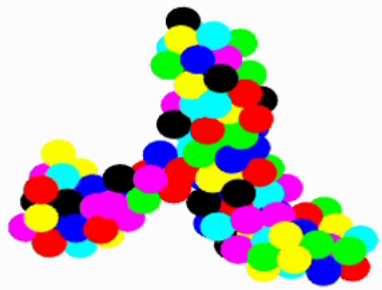

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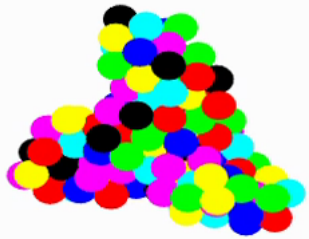


Objective and approach

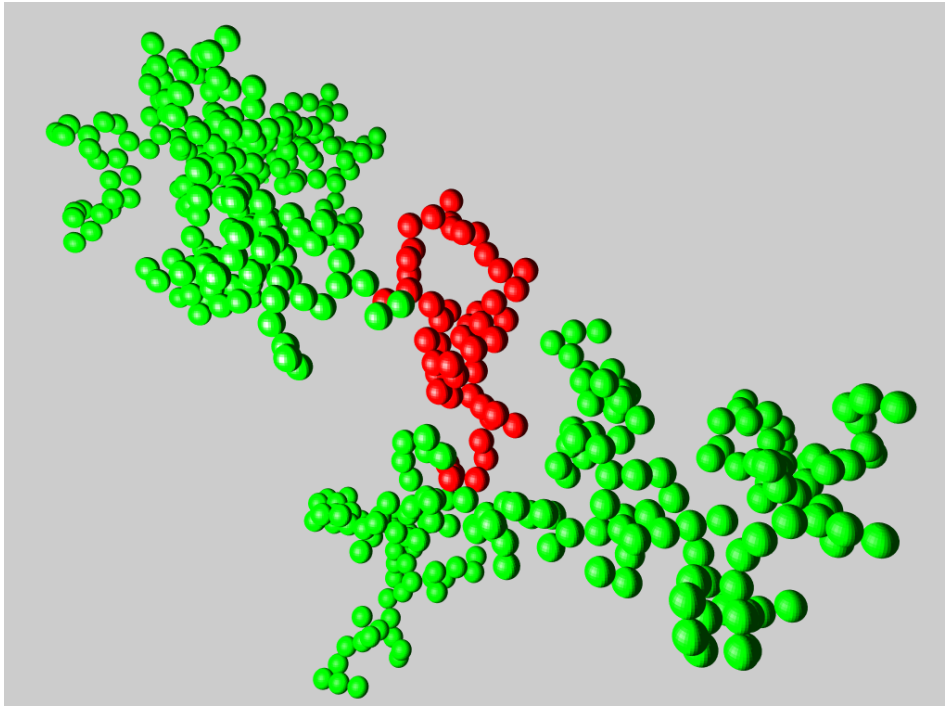
- Objective: derive D_f and k_0 of aggregates of known 3D geometry
- Hypothesis: since aggregates are self-repeating structures, fractal parameters can be estimated by extracting multiple sub-aggregates and performing a linear regression of $\log N$ vs $\log \frac{R_g}{a}$
- Approach: we generate aggregates with a cluster-cluster agglomeration algorithm and determine the optimal way of sampling sub-aggregates to retrieve D_f and k_0 with the greatest accuracy

Key takeaway

Our approach is to use ensemble method with sub-aggregates instead of a collection of different aggregates

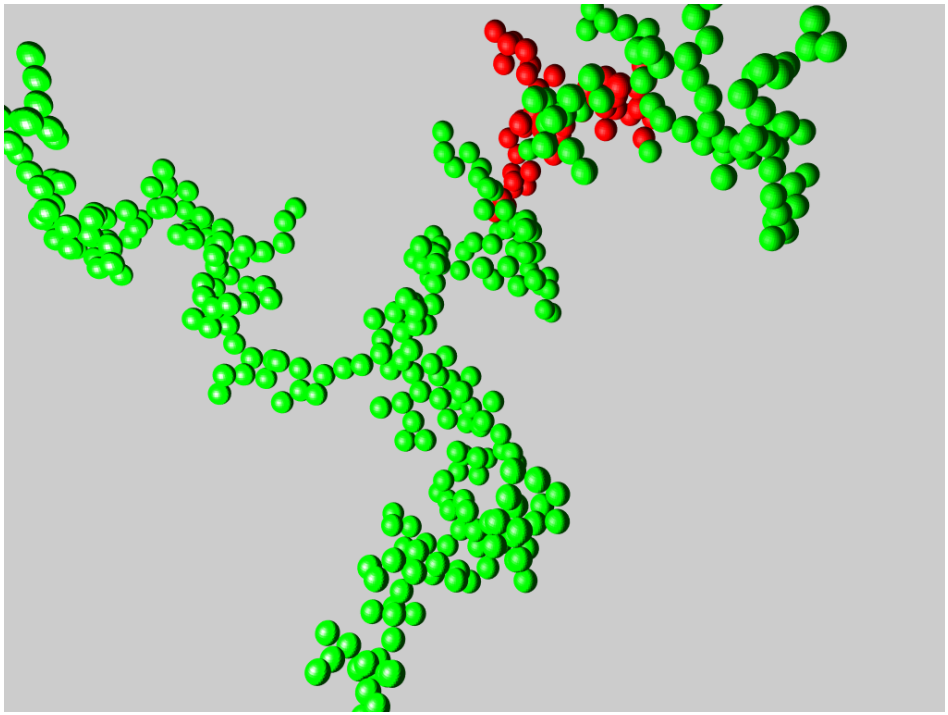
Methodology

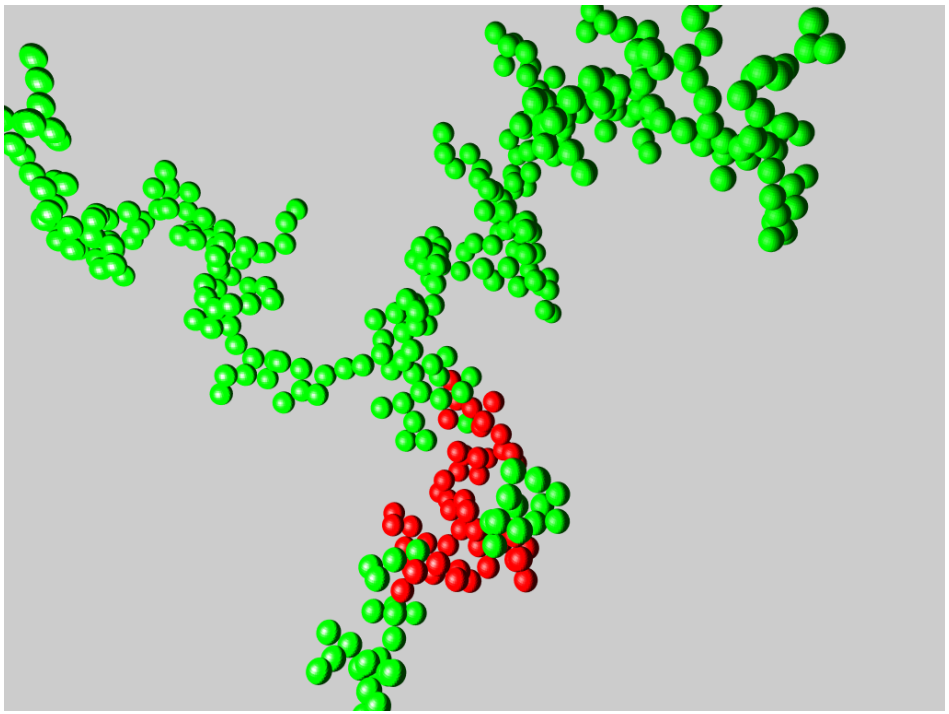
- After an aggregate is generated, a neighbor search is performed on each node to build a topological graph
- To extract a sub-aggregate, a starting node is picked in the aggregate and a sub-aggregate is selected around that starting node
- Radius of gyration of each sub-aggregate is calculated



Aggregate in green ($N = 500$, $k_0 = 1.4$, $D_f = 1.8$) and sub-aggregate in red ($N = 50$)

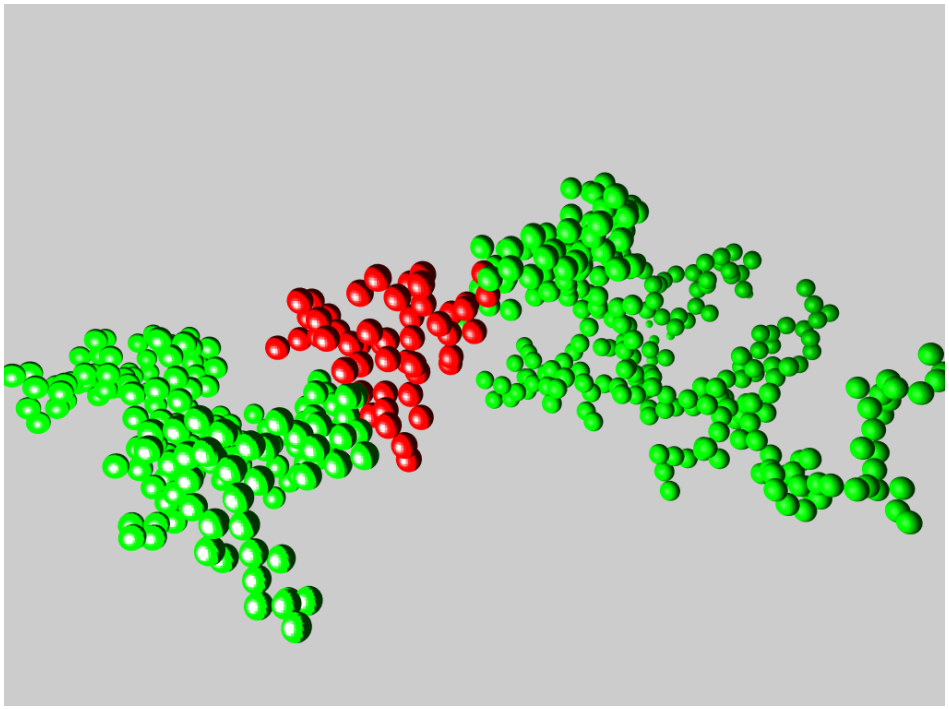
Methodology (continued)

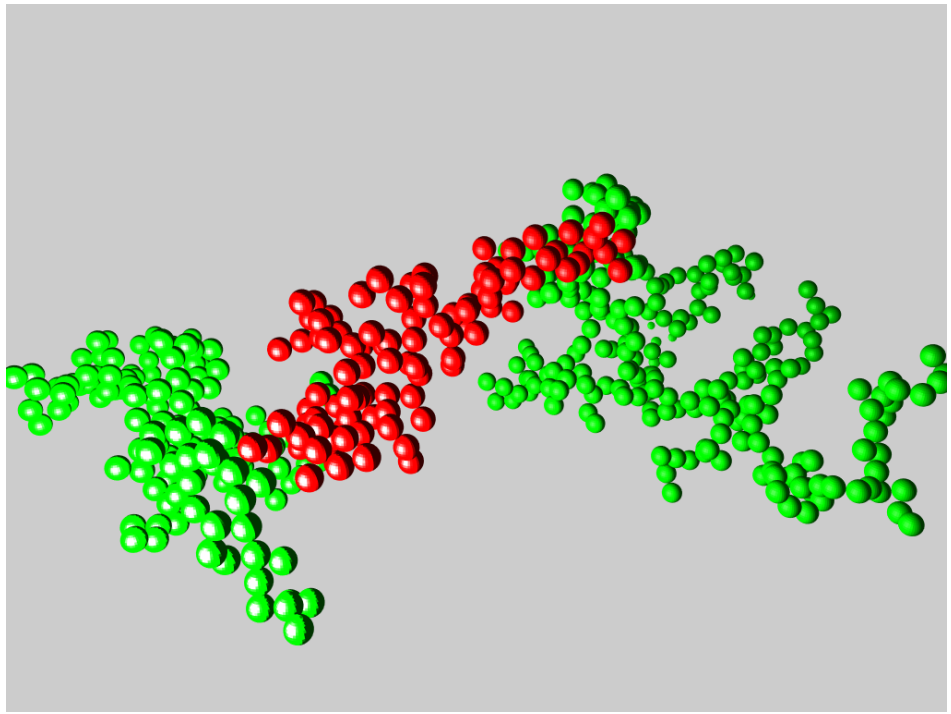




Two sub-aggregates of size $N = 50$ extracted from an aggregate at different locations

Methodology (continued)





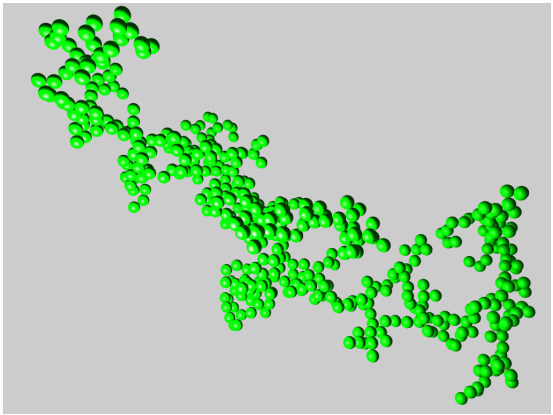
Two sub-aggregates of different sizes ($N = 50$ and $N = 100$) originating at the same point

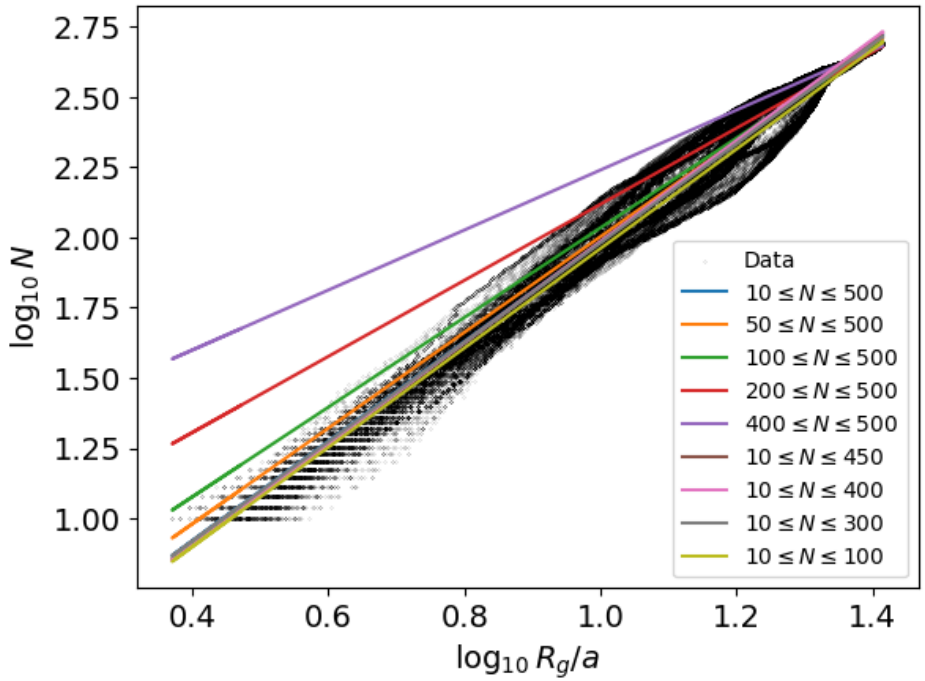
Lacey aggregate analysis

Generated aggregate parameters:
$D_f = 1.80,\ k_0 = 1.40$

Range	D_f	k_0
$10 \le N \le 500$	1.77	1.63
$50 \le N \le 500$	1.70	2.00
$100 \le N \le 500$	1.60	2.75
$200 \le N \le 500$	1.35	5.81
$400 \le N \le 500$	1.07	14.87
$10 \le N \le 450$	1.79	1.57
$10 \le N \le 400$	1.80	1.53
$10 \le N \le 300$	1.77	1.63
$10 \le N \le 100$	1.77	1.56

$$\log N = D_f \log \frac{R_g}{a} + \log k_0$$





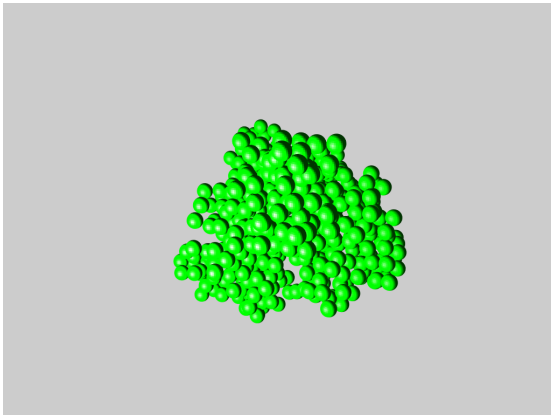
Compact aggregate analysis

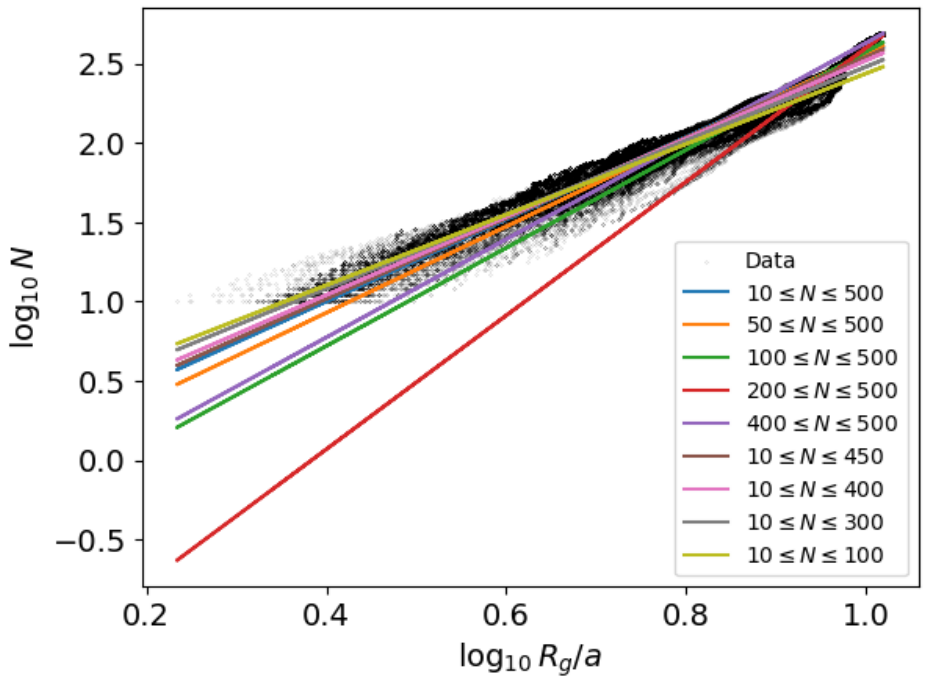
Generated aggregate parameters:

$D_f = 2.50,\ k_0 = 1.40$

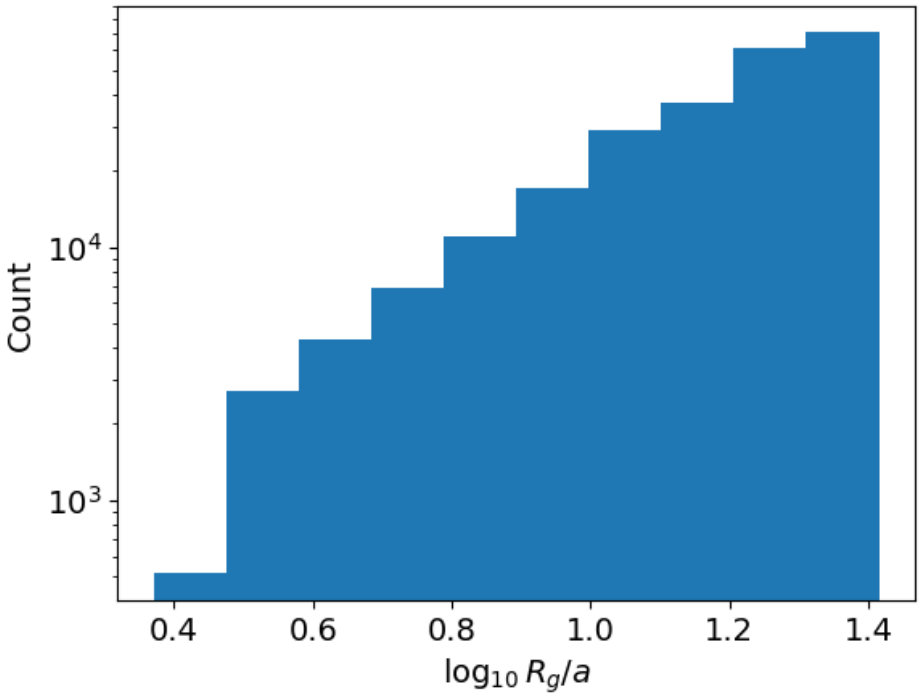
Range	D_f	k_0
$10 \leq N \leq 500$	2.59	0.92
$50 \leq N \leq 500$	2.72	0.69
$100 \leq N \leq 500$	3.09	0.30
$200 \leq N \leq 500$	4.22	0.02
$400 \leq N \leq 500$	3.09	0.34
$10 \leq N \leq 450$	2.54	1.01
$10 \leq N \leq 400$	2.46	1.14
$10 \leq N \leq 300$	2.33	1.41
$10 \leq N \leq 100$	2.22	1.63

$$\log N = D_f \log \frac{R_g}{a} + \log k_0$$

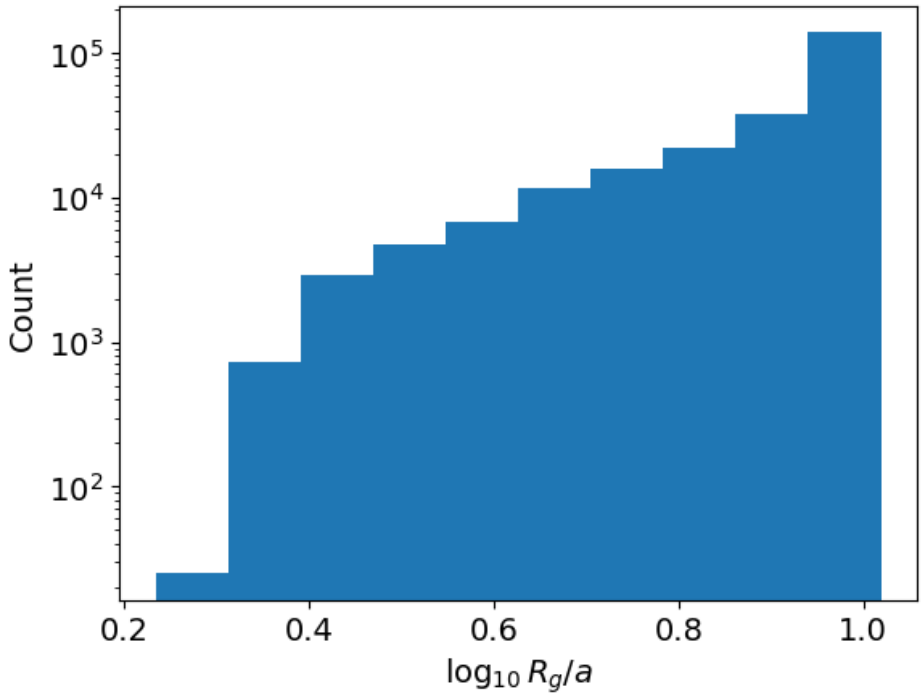




Sampling statistics



Lacey aggregate



Compact aggregate

Key takeaway

Since larger sub-aggregates overlap more, they tend to bias the statistics

Conclusion

- Accuracy of fractal parameter calculation varies based on random aggregate structure
- Using the broadest sub-aggregate size range seems to produce the best outcome
- Increasing the lower bound of the sub-aggregate size range seems to affect the results more than lowering the upper bound
- The algorithm produces reasonable results, which can be improved with further refinement of the algorithm

Key takeaway

Overall, we see the potential of this method to accurately calculate fractal parameters of individual aggregates

Future work

- Improve the sub-aggregate sampling algorithm to reduce the bias of larger sizes:
  - Random sampling (random starting node and sub-aggregate size)
  - Reduce the number of sub-aggregates as their size increases
- Collect statistics from a variety of aggregates with different fractal parameters
- Contain the algorithm in a single library for re-use in further studies

Acknowledgement

Funding

- New Jersey Institute of Technology
- National Science Foundation (award #AGS-1554777)

Software

- Mackowski fractal generation program
- C/C++
  - libglfw
  - libglm
  - libglew
  - libtinyxml
- Python
  - matplotlib
  - numpy