Particle Aggregation Phenomena

Fractals and more!

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Outline

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- Climate Models - important in aerosol science
- Condensation of Stardust
- Cheese Making :)
- Coagulation of Blood and more!

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Fractal math also used: Trading in Stock Markets - *finding order in chaotic price movements*

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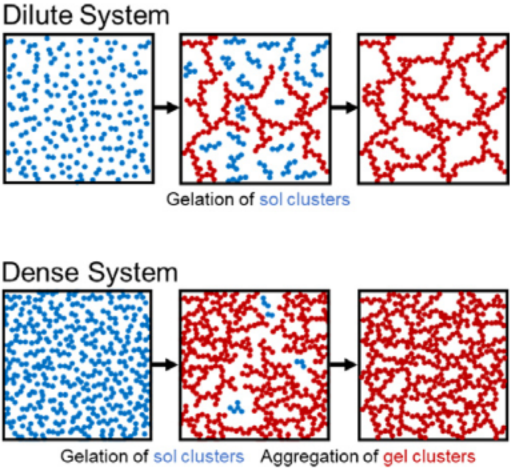
Summary of Particle Aggregation



[1]

[1] Pai Liu et.al., 2019 - My mentors at WashU

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Types of Aggregation Models

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1. Diffusion motion based - (Stochastic)
2. Ballistic motion based - (Deterministic)
3. Reaction limited - (Thermodynamic interactions)

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Mathematical formalism for these dynamically formed clusters

Fractals

Property : "Scalar Invariance"

Figure: Snowflake

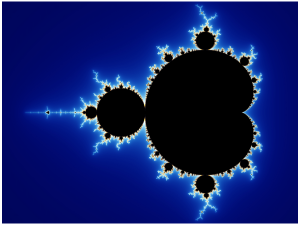

Figure: Mandelbrot Set

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Scaling Law in Fractals

Morphology of aggregates can be summarised by

[2] img from Janusz et al., 2012

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Simple equation

$$N = k_o(R_g/a)^{D_f} \tag{1}$$

Where,

- D_f = Fractal dimension
- k_o = Prefactor info about shape
- N = monomer units in a cluster
- R_g = Radius of gyration
- a = Monomer radius
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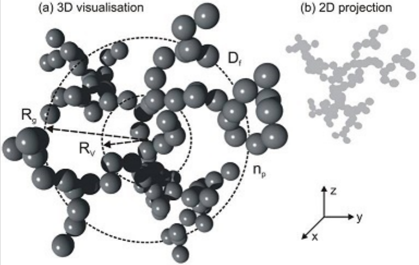

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General notion of Fractal Dimension (D_f)

Observe: $D_f < 3$ (spatial dimension) for 3D aggregates.

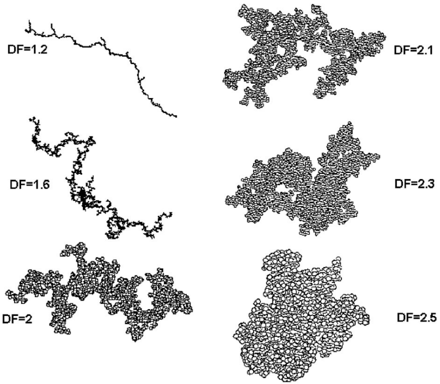

Figure: 2D projections of 3D clusters

[3]

[3] M. Bizi, Natural Science 4 (2012) 372-385

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Theoretical Predictions (from literature)

- Extensive literature on the topic predicts the following scale invariance (D_f).

[4] Martin et al. "Fractal Scaling..", 2014

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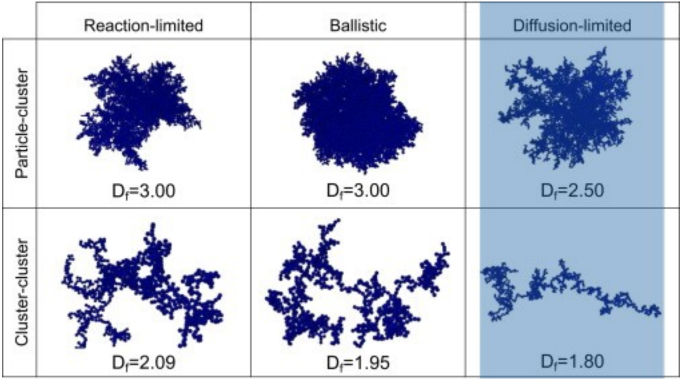

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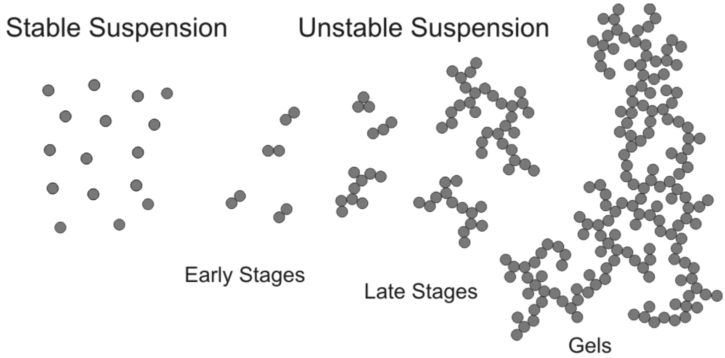


Figure: 2 stages - see next slide for simulation results

Computer Simulations (case study: DLCA)

- $D_f = 1.8$ and $D_f = 2.5$ (best-fit slopes) across different experiments

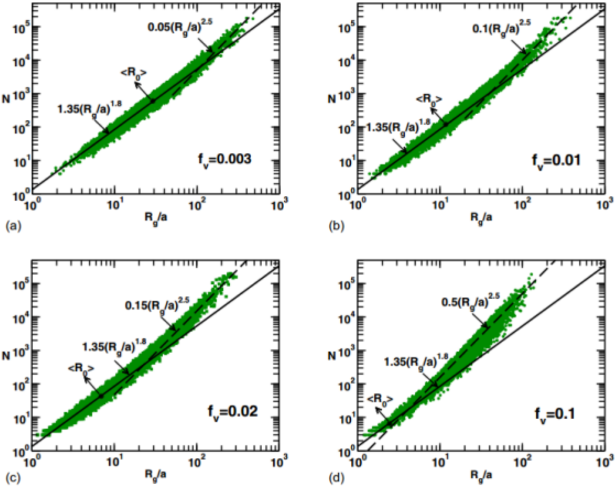
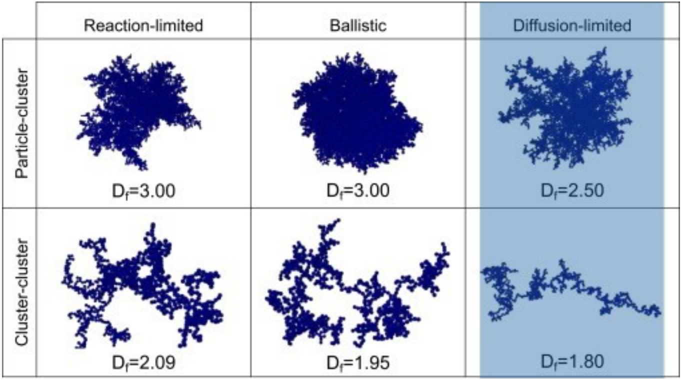


Figure: Snapshots of simulations - various volume fractions

(Repeated) Theoretical Prediction

- Theory is proved my experimental simulations!



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Takeaways

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1. **Fractals** are useful to understand common physical phenomenon such as **Particle Aggregation**
2. Random collisions explained by a fundamental equation similar to the Ideal Gas Law
    - Case study: Scale invariance proved via simulations in a diffusion limited cluster aggregation process (DLCA)
    - $D_f = 1.8$ and $D_f = 2.5$ are common for this process (across different initial conditions)

Outline

Acknowledgements

$\tilde{3}0$ % of Part of my research internship at Washington University in Summer, 2017

Primary articles:

- *The sol to gel transition in irreversible particulate systems*, C. M. Sorensen and A. Chakrabarti, Soft Matter, 2011
- *PhD Dissertation*, William Heinson, 2015
- *Kinetic Percolation*, William Heinson et al, 2017

Appendix

Growth Kinetics Equation - Theory

Growth Kinetics in cluster-cluster aggregation models is described by the Smoluchowski equation (2).

Smoluchowski Equation

$$\frac{dn_N}{dt} = \sum_{i=1}^{N-1} K(i, N-i) n_i n_{N-i} - n_N \sum_{i=1}^{\infty} K(i, N) n_i \tag{2}$$

Here n_i is the number of clusters of size i. The kinetic state of the system is capture in the kernel K(i,j), which is dependent on the present state of the system. i.e time dependence.

Thus Non linearity is introduced into the system.

Langrangian vs Eulerian Perspective

Langrangian :
Viewing the simulation box from a single particle's point of view. i.e. It will be in a frame of reference where it is at rest.

- Cluster-Monomer aggregation as in BA, DLA, RLA

Eulerian :
Viewing the simulation box from outside the box

- Cluster-Cluster Aggregation as in BLCA, DLCA, RLCA

Diffusion Models

- Follow Brownian Dynamics. Also heavier particles move slower
- There are two types:
  1. Diffusion limited monomer-cluster aggregation (DLA).
     - Eg: Coral growth, Coalescing of smoke and dust
  2. Diffusion limited cluster-cluster aggregation (DLCA)
     - Eg: Colloidal aggregation
     - ($D_f = 1.8$ in 3D and 1.4 in 2D).

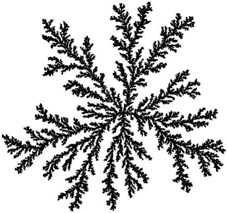

Figure: DLA

Figure: DLCA

Ballistic models

- Deterministic system. Occurs in very low pressure situation or large molecular regime .High Knudsen number(K_n) compared to diffusion scenario.

$$K_n = \frac{\lambda}{L} \tag{3}$$

  where λ = mean free path, L = representative physical length scale
- There are two types:
  1. Ballistic limited monomer-cluster aggregation (BLA). Eg: Thin film growth by vapor deposition
  2. Ballistic limited cluster-cluster aggregation (BLCA). Agrees with theory (D_f=1.91 in 3D and 1.55 in 2D)