Particle Aggregation Phenomena

Fractals and more!

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FCreek Capital - Feb 15, 2020

Outline

Acknowledgements

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

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Nature is complex but the underlying mathematics is beautiful!

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

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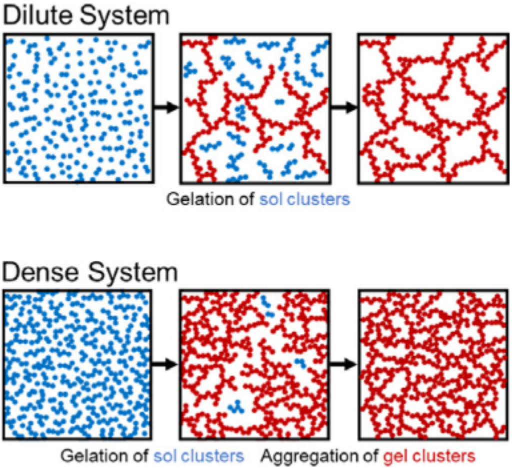
Fractal math is also used for : Trading in Stock Markets - *finding order in chaotic price movements*

Summary of Particle Aggregation



[1]

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

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

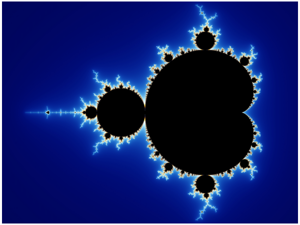

Figure: Mandelbrot Set

Scaling Law in Fractals

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[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
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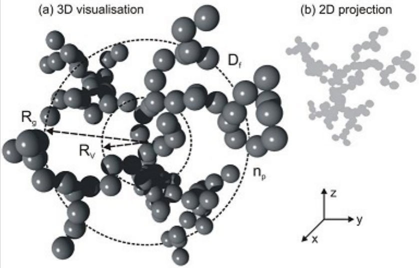

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[2] img from Janusz et al., 2012

General notion of Fractal Dimension (D_f)

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

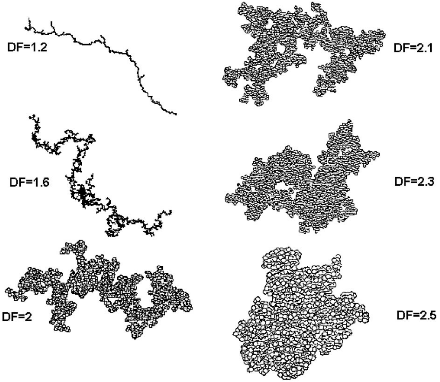

Figure: 2D projections of 3D clusters

[3]

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

Comparison

- I verified the scale invariance (D_f) of diffusion limited process (DLCA) through computer simulations.

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

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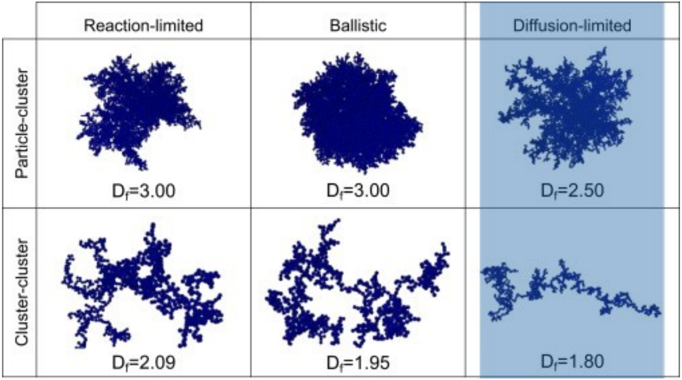

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The Sol-Gel transition-1 (case study: DLCA)

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- Progression of events is as follows

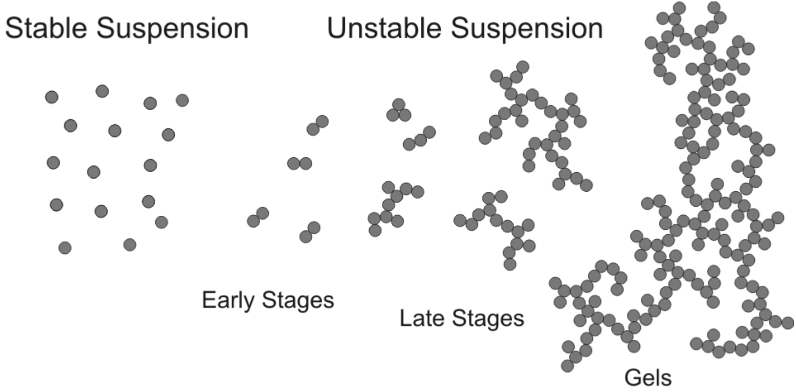

Figure: 2 stages - see next slide for simulation results

The Sol-Gel transition-2 (case study: DLCA)

- Compare this with the scaling equation mentioned earlier

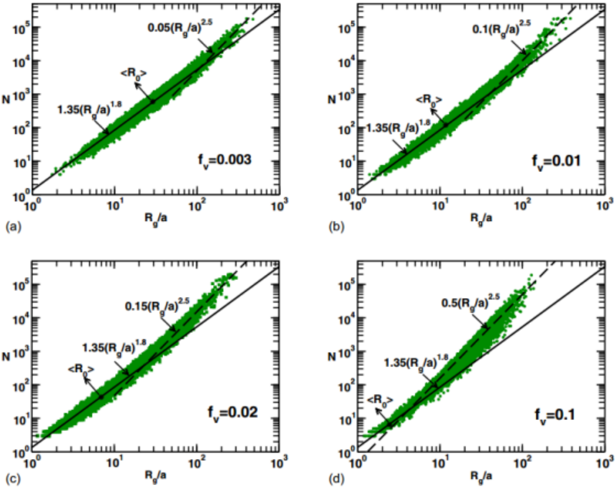

Figure: 2 fixed D_f (slopes of best-fit lines) - various volume fractions

Summary

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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)
   - Initially $D_f = 1.8$ and then $D_f = 2.5$ for this process (across different initial conditions)

Appendix

Growth Kinetics Equation

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).

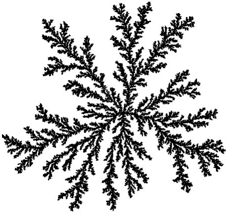

Figure: DLA

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)