Particle Aggregation Phenomena

Fractals and more!

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PH 542 - Nonlinear Dynamics
Aug 30, 2017

Acknowledgements

- *PhD Dissertation*, William Heinson, 2015
- *The sol to gel transition in irreversible particulate systems*, C. M. Sorensen and A. Chakrabarti, Soft Matter, 2011, 7, 22842296
- *Kinetic Percolation*, William Heinson et al, 2017
- Few images from Google image search. It will be mentioned in the presentation.
- Wikipedia articles for key concepts
- Credit for other work is given in the slides itself

Outline

Why this topic?

Particle aggregation is a widely observed phenomenon in many seemingly unrelated fields.

Application areas

- Climate models- Very important in Aerosol science
- Condensation of stardust
- Colloidal particle dynamics
- Sol-Gel Transition
- Formation of River Delta
- Cheese Making :)
- Coagulation of blood and more!

Types of Aggregation Models

- Diffusion based Models - (Stochastic)
- Ballistic motion based Models - (Deterministic, except for initial random motions)
- Reaction Limited Model - (Slower version of DA with slight changes in thermodynamic interactions)

If we look at each model, One thing is common i.e. the way we describe the dynamically formed clusters - Fractals

Fractals have very important implications in the fields of both reversible and irreversible aggregation. The equations involved are usually very complex and many factors simultaneously affect the process.

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

Scaling Law

The compact equation (1) is known as the Scaling equation for aggregates which gives compact information about aggregates or clusters or agglomerates.

Equation

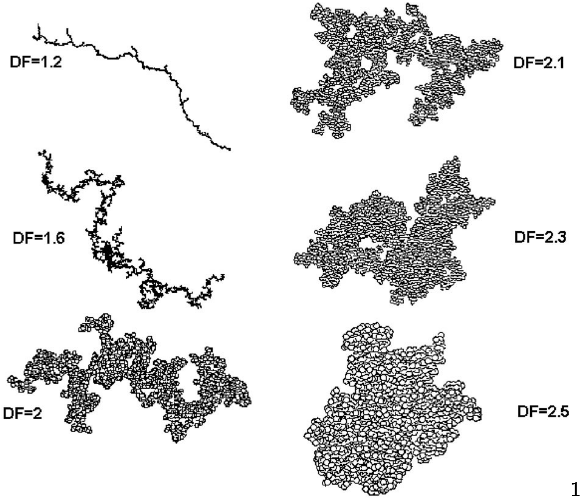
$$N = k_o(Rg/a)^{D_f} \tag{1}$$

Where,

- Df = Fractal dimension
- ko = Prefactor Info about shape
- N = Number of monomer units in cluster
- Rg = Radius of gyration, a= Monomer radius

General notion of Fractal dimension (Df)

This is a 2D projection of 3D aggregates.



[1]

[1] Source- DOI:10.4236/ns.2012.46052

Diffusion Models

- Follow Brownian dynamics. Also heavier particles move slower
- There are two types:
  1. Diffusion limited monomer-cluster aggregation (DLA). Eg: Zinc ions in electrolyte near electrodes, Coral growth, Coalescing of smoke and dust.
  2. Diffusion limited cluster-cluster aggregation (DLCA) Eg: Developed from DLA and works well for colloidal aggregation. Agrees with theory (D_f=1.78in 3D and 1.44 in 2D).

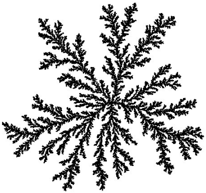


Figure: DLA

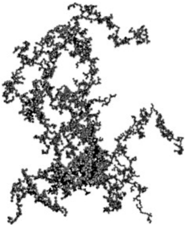


Figure: DLCA

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.

Ballistic models

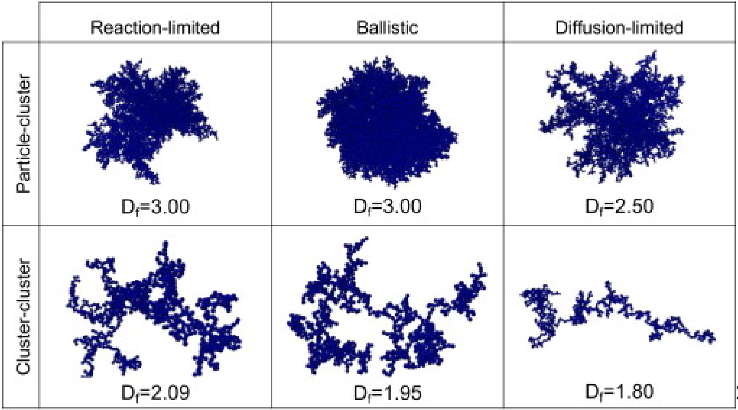
- Deterministic system. Occurs in very low pressure situation or large molecular regime .High Knudsen number(K_n) compared to diffusion scenario.

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

  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)

Comparison

- Look at the comparison between clusters formed through the different paths



[2]

[2]source: https://doi.org/10.1016/j.ces.2014.03.024

Time for simulations

- Observe the following simulations done by us. The python code required for simulating it was relatively simple.
- Parameters such as velocity of motion and number of particles in the system, etc affect the dynamics of the system.
- Transitions from one mode to another in the same simulation system are seen!

Chaos in ballistic aggregation ?

Something to ponder over.

- In ballistic motion, We are sure of the path each particle takes after every collision
- Does this mean the system is deterministic ?
- Does slight change in initial conditions cause irreversible loss in predictability (subtly mentioning chaos)?

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If fractal self similarity is necessary for chaos, Ballistic motion produced fractals are self affine. Hence we reject the notion of chaos here.

The Sol-Gel transition-1

- Progression of events is as follows

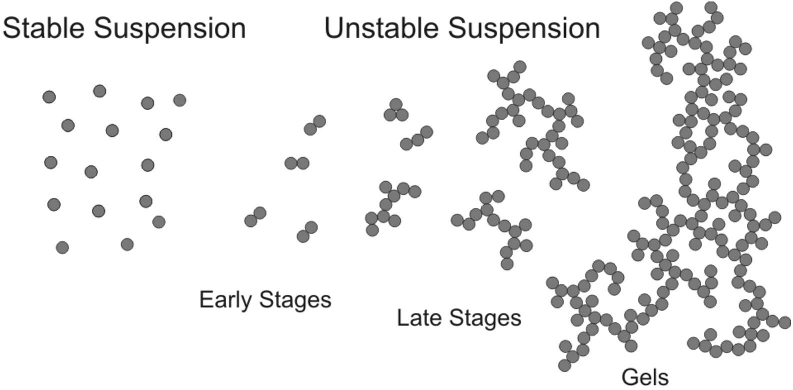

Figure: Stable vs. Unstable systems

The Sol-Gel transition-2

- Compare this with the scaling equation mentioned earlier

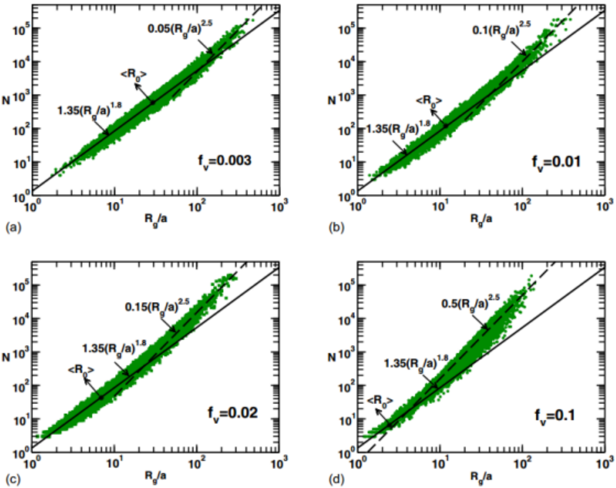

Figure: Look at how Df (slope of line) varies

Summary

- To stress the fact that fractals are really useful to explain things which seem too complex otherwise.
- We observe that in free molecular regime individual particles become irrelevant during this active, interactive process.
- Random collision interactions between particles gives rise to something fundamental with a unique parameter (ex: Df = 1.8 for 3D DLCA process) across multiple processes.
- Overall picture from a concatenated (in time) point of view makes more sense in stochastic simulations (fig 4)
- Outlook
  - Our Proposition is that given infinite amount of time any closed system will eventually attain fully gelled state (Tough to prove!).
  - We think that ballistic does not show chaos.

Any more questions?
Thank you