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3D simulation of the Cluster–Cluster Aggregation model☆

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ABSTRACT

We write a program to implement the Cluster–Cluster Aggregation (CCA) model with java programming language. By using the simulation program, the fractal aggregation growth process can be displayed dynamically in the form of a three-dimensional (3D) figure. Meanwhile, the related kinetics data of aggregation simulation can be also recorded dynamically. Compared to the traditional programs, the program has better real-time performance and is more helpful to observe the fractal growth process, which contributes to the scientific study in fractal aggregation. Besides, because of adopting java programming language, the program has very good cross-platform performance.

Program summary

Program title: CCA

Catalogue identifier: AEUK_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEUK_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html

No. of lines in distributed program, including test data, etc.: 390649

No. of bytes in distributed program, including test data, etc.: 83881850

Distribution format: tar.gz

Programming language: Java.

Computer: Any computer with Windows, java jdk and java3d jdk installed.

Operating system: Windows.

RAM: Determined by the number of the initial particles in the simulation test

Classification: 14, 16.12.

Nature of problem:
The programs for the CCA model published are very rare, and are mostly in the form of a 2D figure. So, existing computer simulation programs cannot well simulate the fractal aggregation. Compared to the existing programs, our simulation program for the CCA model in the form of a 3D figure can better simulate the process dynamically.

Solution method:
A program is provided that well simulates CCA model in the form of a 3D figure. The program implementation is based on the java programming language. Especially, we use the java3d technology to display the simulative graphics in form of 3D.

Restrictions:
In order to show the process of fractal aggregation growth dynamically, this program needs to refresh the graphics of aggregation of colloidal particle frequently. So this program takes up a lot of computer

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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memory. The storage capacity of the computer memory used to run the program will limit the number of single particles which the program can simulate.

Unusual features:
The program simulates the CCA model in the form of a 3D figure using the java3d technology.

Additional comments:
!!!!Due to the large file size, CCA is not delivered directly when download or Email is requested. Instead an html file giving details of how the program can be obtained is sent.!!!!

Running time:
Determined by the size of the problem.

1. Introduction

Fractal aggregation is a frontier topic in the study of nonlinear science, which has been widely applied to physical, chemical science and social science. There are a lot of models for studying fractal aggregation, such as Diffusion-Limited Aggregation (DLA) model, Ballistic Aggregation (BA) model, Reaction-Limited Aggregation (RLA) model, Cluster–Cluster Aggregation (CCA) model [1–5]. The CCA model is put forward by Meakin and Kolbon, which is on the background of the aggregation of the dusts in the atmosphere and colloidal particles [6–8]. The CCA model assumes that initially a collection of equal sized individual spherical particles are randomly dispersed in a box at low concentrations and then these particles are allowed to self-diffuse in Brownian motion by random walk, collide, and form clusters [4,5]. Fractal aggregation is an important physical and chemical process, it is a common natural phenomena and also plays an important role in industrial production. So CCA models have a wide range of practical application possibilities.

With the development of computer technology, computer simulation becomes a more and more significant method for research on fractal aggregation. However, the existing programs to realize CCA model are few and most of them are in the form of two-dimensional (2D) figures. The program can dynamically display the growth process of fractal aggregation in the form of a three-dimensional (3D) figure. Thus the simulation is closer to the real fractal aggregation phenomenon in the nature and more conducive to the scientific study in fractal aspect. Meanwhile, the program is implemented by java program language, so the program has very good cross-platform performance, and is simple and convenient for users.

2. The mechanism of CCA model

When realizing the simulation for CCA model, the main work is to realize the simulation of particles' or clusters' Brownian motion, collision detection and aggregation [9]. The following is the conventional algorithm of the CCA model in Fig. 1.

Firstly, all the particles are randomly distributed in a cubic box with side-length L. When the particle concentration C is given, the number of all the single particles N can be obtained by the following formula:

$$N = C * L^3. \tag{1}$$

During the process of Brownian motion, one particle or cluster will be selected in each step for a potential movement. The selection is accepted or rejected based on the probability P_{move} [4,10]:

$$P_{move} = D_i/D_{\max} \tag{2}$$

$$D_i = D_1 \times S^r \tag{3}$$

where D_i is the diffusion coefficient of the cluster consisting of i particles, D_{max} is the maximum diffusion coefficient for any cluster in the system. For the potential movement, a random number x uniformly distributed over the range [0, 1] is generated and the cluster is moved only if $x < P_{move}$. S is the mass of cluster, which is expressed by the number of the particles contained in the clusters in the practical application. r is the diffusivity exponent. D_1 is the diffusion coefficient of the single particle and its calculation formula can be derived according to Einstein's diffusion law, as follows:

$$D_1 = k/f \times T \tag{4}$$

where k is Boltzmann constant and its value is $1.3806503 \times 10^{-23}$ J K^{-1}, f is coefficient of friction and T is the absolute temperature of the experimental system.

In the process of moving, the selected cluster can move to six directions (up, down, left, right, front and back). For each moving step, the moving direction is randomly chosen among the six directions. After the selected cluster moves a step, if the selected cluster does not collide with another one, the displacement is performed and the algorithm goes on by choosing another cluster. For the next step, if a collision occurs between two clusters (one consists of i particles, and another consists of j particles) they stick together forming a new larger cluster with the sticking probability P_{ij} [4,11]:

$$P_{ij} = P_1 \times (i \times j)^{\sigma} \tag{5}$$

where P_1 is the sticking probability of single particles, σ is the sticking probability exponent.

In the process of collision simulation, a random number y uniformly distributed over the range of 0 to 1 is generated and compared with the calculated P_{ij}. The sticking is considered effective only when $y < P_{ij}$ is verified.

3. The computer simulation realization of CCA model

We have completed the simulation program for CCA model with java language. Fig. 2 shows the situation of running the program.

There are six parameters as the initial conditions in the interface of the simulative program. We can set different values for each parameter according to different research goals. The descriptions of these parameters in detail are as follows:

Parameter L is the side-length of the cubic box and parameter C is the particle concentration. The total number of particles is determined by these two parameters. Displaying the CCA simulation result in the form of a 3D figure needs to take up a lot of computer memory, so the number of particles the program can simulate depends on the capacity of the computers' memory used to run the program. By doing the simulation experiment many times, we find that the program can simulate around ten thousand particles under the condition that the computer has a 2G memory, and when