Space-time growth-interaction processes with moving objects versus the force biased algorithm

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Background

- Jodrey and Tory (1981, 1985, 1986): Force biased (FB) algorithm for generating random close packings of balls from a random distribution of balls
- Ballani, Daley and Stoyan (2006): Model the microstructure of concrete by the FB algorithm
  Lautensack, Schladitz and Särkkä (2006): Model the microstructure of sintered copper by the FB algorithm
  → FB too regular compared to data
  → random shifts
- Renshaw and Comas (2008): Use growth-interaction processes to generate high intensity patterns
- Lautensack, Renshaw and Särkkä: Would growth-interaction processes be able to produce more realistic sintered copper (and other) patterns?

Outline

- Force biased algorithm
- Immigration-growth spatial interaction process with moving particles
- Immigration-growth versus immigration-growth with movement (IGM)
- IGM versus FB
- Conclusions/Future work

Force biased algorithm

Start with a configuration of n balls $b(x_i, \frac{d_i}{2})$ with diameter d_i centered at x_i, $i = 1, ..., n$

Each ball is given an inner diameter and an outer diameter

- The inner diameter is chosen so that there are no overlaps in the system and exactly two balls are in contact
- The outer diameter is calculated based on the desired volume fraction and the diameter of the ball

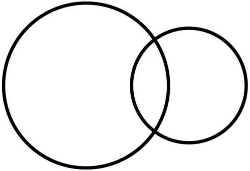
Force biased algorithm

The algorithm attempts to reduce overlaps between the balls in every step by two operations

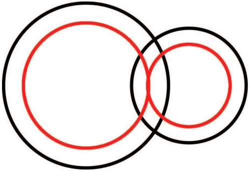
- pushing apart the overlapping balls by choosing new positions (repulsion force and potential function introduced)
- gradually shrinking the balls by reducing the outer diameter

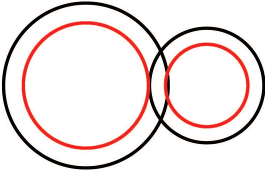
The two diameters approach each other and the algorithm stops when the inner diameter becomes greater or equal to the outer diameter

Force biased algorithm: Starting configuration

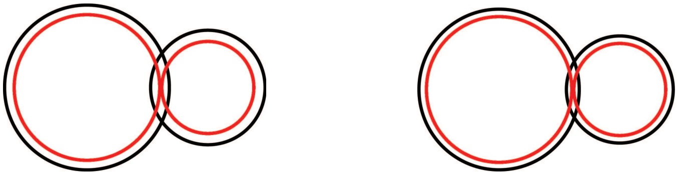


Force biased algorithm: Scaling and moving





Force biased algorithm: Expanding and shrinking



Force biased algorithm

- The algorithm generates packings in which only two balls are in contact but many balls are nearly touching
- Reorganizes the initial pattern, randomness comes from the initial configuration
- Tends to produce very regular patterns
- Would it be possible to produce patterns with larger variety by using the space-time growth-interaction process?

Immigration-growth-spatial interaction process

New immigrants arrive according to a Poisson process, with rate α, have uniformly distributed locations, and are assigned some marks

In small time intervals $(t, t + dt)$, each individual either dies 'naturally' with probability μdt, or undergoes the deterministic size change

$$\begin{aligned} m_i(t+dt) &= m_i(t) + f(m_i(t))dt \\ &+ \sum_{j \neq i} h(m_i(t), m_j(t), \|x_i - x_j\|)dt, \end{aligned}$$

where

$f(\cdot)$ individual growth function

$h(\cdot)$ spatial interaction function

$\|x_i - x_j\|$ distance between ball centers i and j

Immigration-growth-spatial interaction process with moving balls

Advantages of moving the balls

- without movement the maximum packing density rarely reaches 50%
- since balls can become smaller they are able to squeeze through small gaps from areas with high intensity to areas with low intensity of balls

Comas and Mateu (2006) and Renshaw and Comas (2008) have suggested some movement strategies.

Moving balls following Renshaw and Comas

During the small time increment $(t, t + dt)$, the position of the ball is perturbed and the particles are moved according to the formula

$$x_i(t + dt) = x_i(t) + v \sum_{j \sim i} \min\{1, m_j(t)/m_i(t)\} \frac{x_i(t) - x_j(t)}{\|x_i(t) - x_j(t)\|},$$

where v is velocity and the sum is over all balls that interact (overlap) with (x_i, m_i).

Immigration-growth-spatial interaction process, where the particles grow according to

$$\begin{aligned} m_i(t+dt) &= m_i(t) + \lambda m_i(t)(1 - m_i(t)/K)dt \\ &\quad - b\sum_{j\neq i} \mathbf{1}(\|x_i - x_j\| < r(m_i + m_j))dt, \end{aligned}$$

where λ is the growth rate, K the carrying capasity, b the strength of interaction and r the range of interaction, and move according to

$$x_i(t+dt) = x_i(t) + v\sum_{j\sim i} \min\{1, m_j(t)/m_i(t)\} \frac{x_i(t) - x_j(t)}{\|x_i(t) - x_j(t)\|},$$

Illustration: simulation

- fixed number of points, here 1000 (α not needed)
- $\mu = 0$ (points die only due to competition)
- new immigrants placed only within empty space
- initial mark size fixed (instead of random), $M_{init} = 0.05$
- $\lambda = 1$, $K = 0.1$ and $r = 1$
- we let v and b vary

Force biased versus immigration-growth-movement

- In FB randomness comes from the initial configuration only, in IGM also from arrival and death
- In FB scaling is global, in IGM we have individual growth
- In FB relative size of the balls does not change, in IGM large balls may become small and vice versa
- Balls move according to $x_i(t+dt) = x_i(t) + \sum_{j\sim i} F_{ij}$, where the repulsion force F_{ij} is

$$F_{ij} = \frac{1}{2d_i}\rho p_{ij}\frac{x_i(t)-x_j(t)}{||x_i(t)-x_j(t)||}$$

(scaling factor ρ and potential function p_{ij}) and

$$F_{ij} = v\min\{1, \frac{m_j(t)}{m_i(t)}\}\frac{x_i(t)-x_j(t)}{||x_i(t)-x_j(t)||}$$

for FB and IGM, respectively

Force biased versus immigration-growth-movement: simulation

- 3D simulations of IGM in the unit cube
- Small balls (growth rate λ_1) and large balls (growth rate λ_2), logistic growth function and symmetric interaction function
- Volume fraction computed from these images
- FB packings simulated with the volume fraction and the radii of the balls in the IGM images (also with random shifts)
- Different statistics plotted in order to compare the realizations

Conclusions

- The patterns produced by FB and IGM differ from each other
- FB with shift and IGM are more similar to each other than FB and IGM (coordination number), but some differences still exist (nearest neighbour distance function, correlation functions)
- IGM may be able to produce a larger variety of patterns
- We can give the desired size distribution to FB but not to IGM

Future work

- Can we write FB as a special case of IGM?
- How to control the size distribution in IGM?
- How to measure the pattern structure? New summary statistics?