Modeling the Packing of Nano-Powders

N. Topić[1], D.E. Wolf[2] and T. Pöschel[1]
[1]Institute for Multiscale Simulations of Particulate Systems, Universität Erlangen-Nürnberg
[2]Institute for Computational and Statistical Physics, Universität Duisburg-Essen

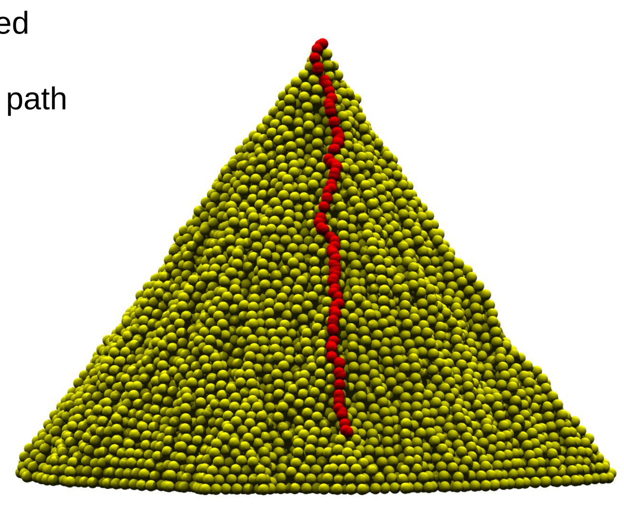
Deposition of particles onto a solid surface appears in many scenarios in engineering and science. Various simple models have been used to gain deeper understanding of phenomena appearing in experiments. In particular, the ballistic deposition algorithm has been used to study packing characteristics, fractal properties and surface roughening in deposits of particles. Here, we present a generalization of a ballistic deposition algorithm to complex particles composed of spheres. Using this generalized algorithm as a model for dynamics of agglomerates of nanoparticles, we show that nanopowders develop a robust fractal substructure after repeated fragmentation and reagglomeration.

Visscher Bolsterli model

The model by W. Visscher and M. Bolsterli describes the deposition of spherical particles within a gravity field.

Assumptions:
- Particles are dropped one by one
- They follow the path of steepest descent
- They stick at stable position

The red particle is dropped from the top the heap. It follows steepest descent path until it reaches a stable position where it sticks.

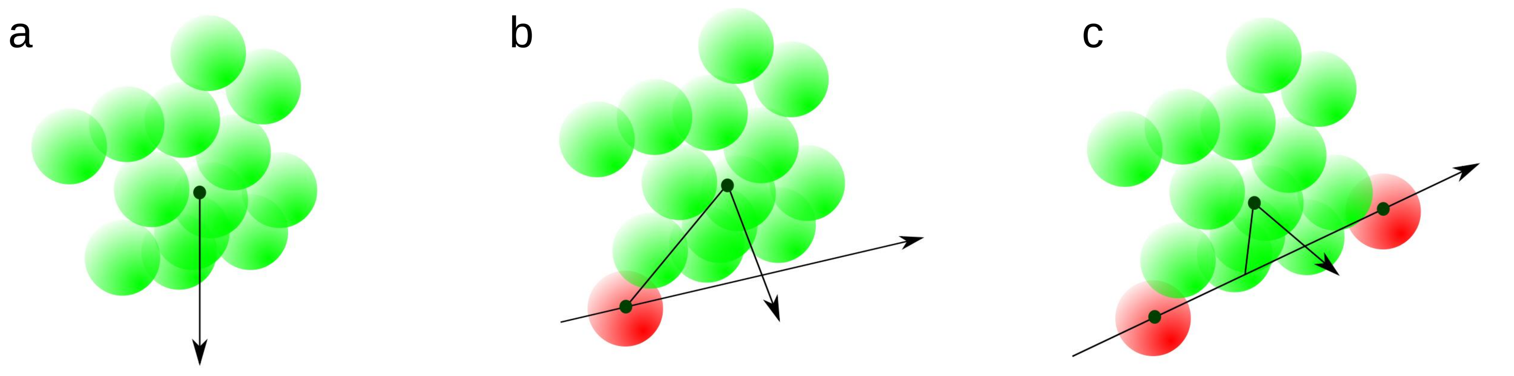


Single particle dynamics is composed of the motion on a straight straight line (falling) and rotation (rolling). Since equations for contacts between particles can be solved analytically this model can be implemented in an event – driven way.

Tens of millions of particles can be simulated

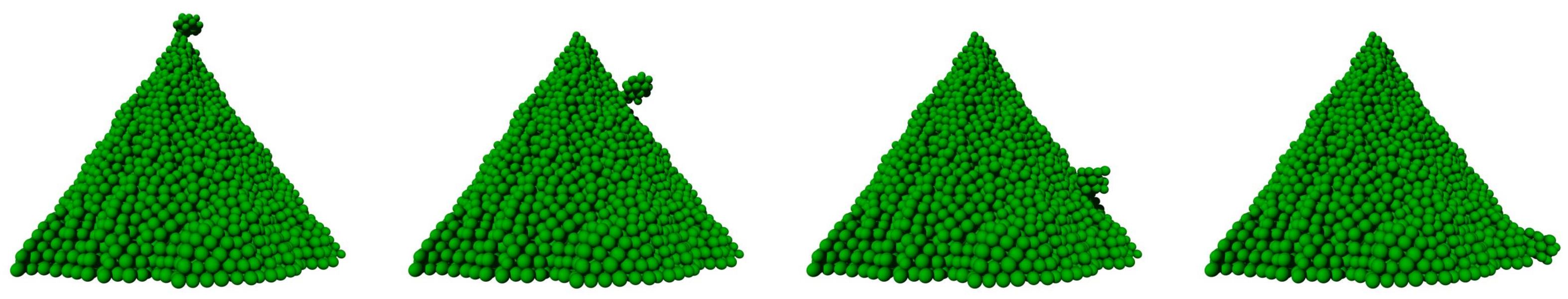
Generalization to complex particles

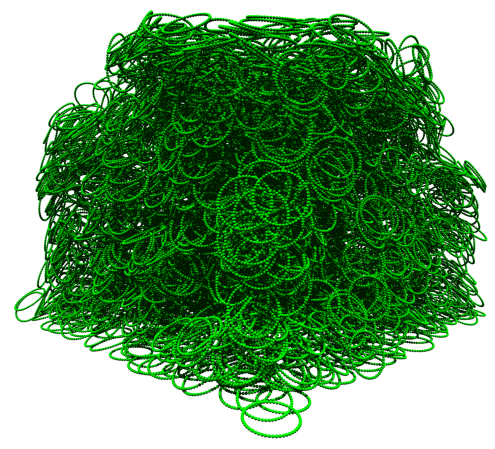
Trajectory of complex particle rolling on a deposit composed of spheres can not be solved analytically. In order to avoid numerical integration of equation, we make approximation that a particle dynamics is composed of two motions: vertical falling and rotation around contacts. As in the original algorithm dynamics is over-damped (inertial effects are neglected).

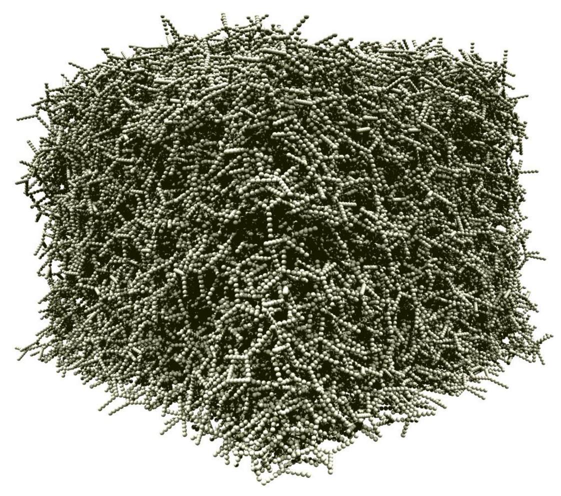


Description of the dynamics: a) When particle has no contacts it falls vertically, b) With one contact particle rotates around the axis through the center of the contacting particle. This axis is perpendicular to vertical and vector joining center of mass and center of contact particle. c) Particle rotates around the axis through centers of contacting particles.

Example of particle motion:







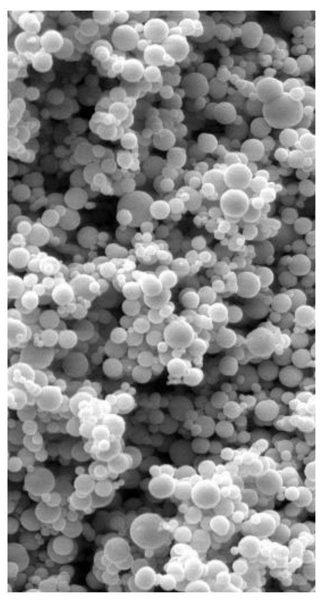
Application: Asymptotic structure of nanopowders

Idea

For nanoparticles van der Waals forces are much stronger than their weight. Due to those forces agglomerates of nanoparticles form very porous and often fractal structures

Nanopowders are treated with various perturbations: shaking, pouring, stirring etc.

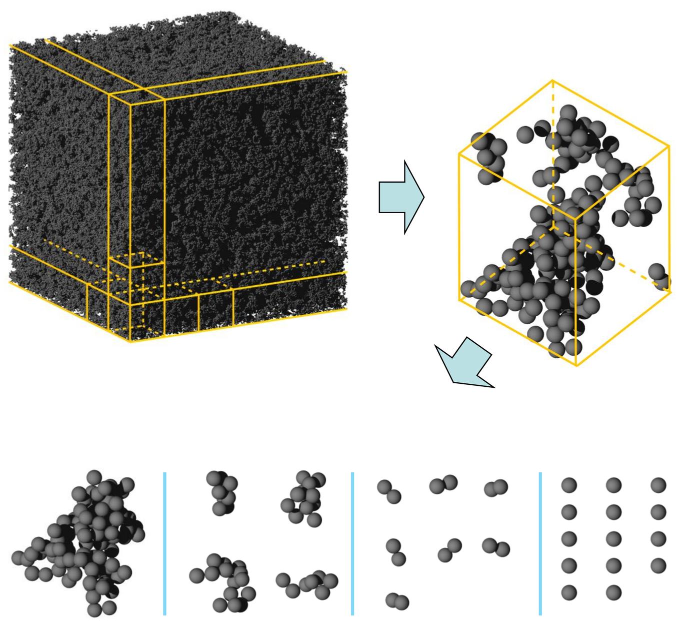
Question: Is there an asymptotic structure invariant to repeated fragmentation/deposition?



Morgeneyer et al.'06
Carboxyl-Iron powder
d=1.94 µm

Fragmentation

Each random treatment breaks the nanopowder into fragments of typical size determined by the prevailing shear forces. We model this fragmentation by cutting with qubic mesh.



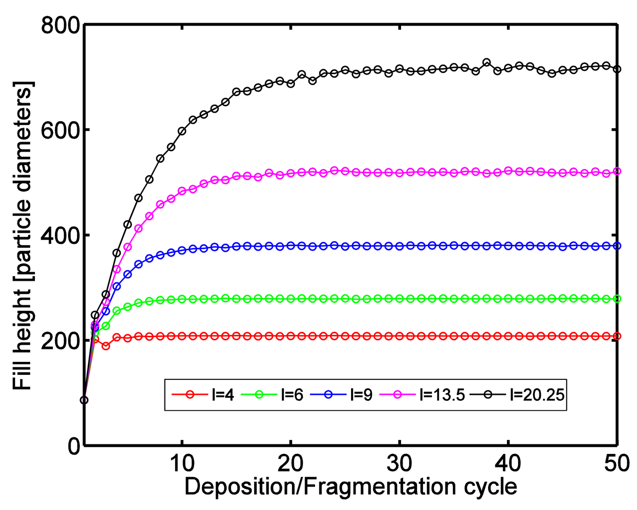
Deposition

Fragments made up of nanoparticles have the following properties:
- They move approximately as rigid bodies
- The fragment weight is larger than the van der Waals forces
- Brownian motion can be neglected due to their size
- The dynamics of nanoparticle flakes is usually strongly damped

Steepest descent model is a reasonable approximation

Existance of asymptotic structure

We perform repeated deposition and fragmentation within a box periodic in x and y directions. Evolution of filling height of deposit with number of deposition/fragmentation cycles is shown on the figure on the right. Each curve corresponds to a different fragmentation length l. Procedure starts from a densely packed powder. After certain number of cycles the filling height becomes invariant. This suggests that a stationary structure has been reached.



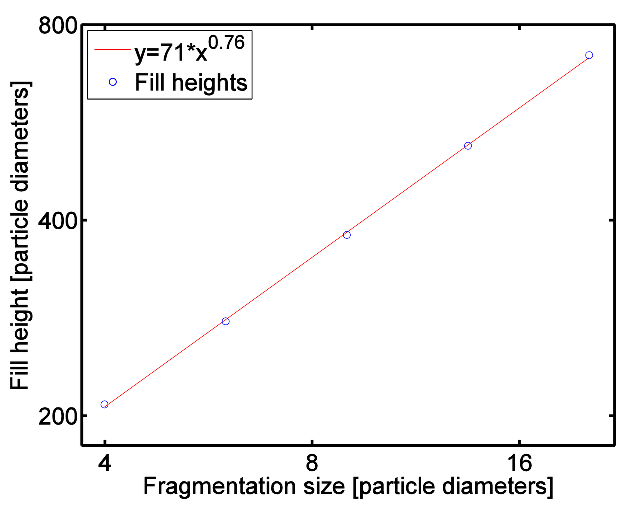
Dependance of asymptotic fill height on fragmentation length

The asymptotic filling height, h(l), as a function of fragmentation length can be fitted very well with a power law:

$$h(l) \sim l^{\alpha}$$

With the exponent:

$$\alpha = 0.76$$



Fractal structure

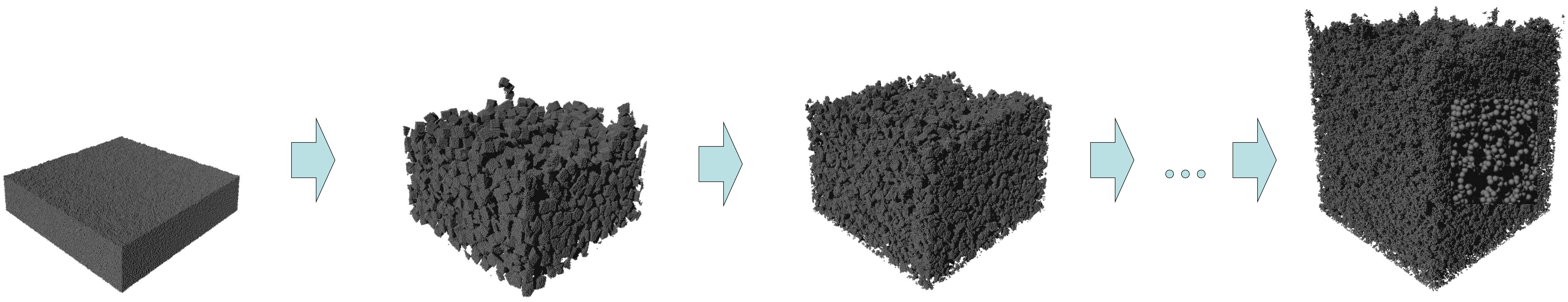
Dependance of mass on l in each of the fragmentation cells gives the fractal dimension [3]:

$$M/N_p \sim l^{d_f}$$

The total numer of cells is: $N_p = L^2 h(l)/l^3 \sim l^{\alpha-3}$

Therefore the fractal dimension is: $d_f = 3 - \alpha = 2.24$

Asymptotic structure is fractal!
(up to fragmentation length)



References:

[1] W. M. Visscher and M. Bolsterli, Nature **239**, 504 (1972).
[2] T. Schwager, D.E. Wolf, T. Pöschel, Phys. Rev. Lett. **100**, 218002 (2008)
[3] Strictly speaking this is true only if short range structure is independent of l. This was shown for 2D systems ([2]). We assume that this is also correct in 3D.

We generalized the steepest descent ballistic deposition model to case of complex particles composed of spheres. Our algorithm was used as a model for dynamics of agglomerates of nanoparticles. Using this dynamics it was shown that nanopowders develop a robust fractal substructure after repeated fragmentation and reagglomeration.