Dynamics of Dust Aggregates

Wilhelm Kley & Alexander Seizinger

Institut für Astronomie & Astrophysik & Kepler Center for Astro and Particle Physics Tübingen







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Dust Dynamics



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Coagulation of Dust & Accretion of Gas (99% Gas, 1% Dust)



Growth: Dust \Rightarrow Planets (μ m \Rightarrow 1000km) (Mass Growth of 35 orders of Magnitude)

Original Matter:

- Oxides, silicates, organic material, ice

Size: μ m

Dust Particles condense in Disk

Growth by :

- Sequence of Collisions & coagulations



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Context Ingredients I

1) Interstellar Dust Measure interstellare Extinction Size distribution (MRN) $n(a) \propto a^{-3.5}$





"Sure it's beautiful, but I can't help thinking about all that interstellar dust out there."

(Mathis, Rumpl, Nordsieck, 1977)

Context Ingredients II

2) Protoplanetary Disk

MMSN: Minimum Mass Solar Nebula

- Augment planet mass with Gas to solar abundance
- split into rings
- spread material therein

$$\Sigma(r) \approx 1700 \left(\frac{r}{1AE}\right)^{-3/2} \mathrm{g/cm}^2$$

(Hayashi, 1981)

Total Mass:

 $\approx 0.01 - 0.07 M_{\odot}$

total angular momentum:

 $\approx 3 \cdot 10^{51} - 2 \cdot 10^{52} \text{ g cm}^2 \text{ s}^{-1}$

typical model for protoplanetary disks



(Weidenschilling, 1977)

(1)

Context Particle Dynamics in Disk

Particles need relative Velocity for mutual collisions Causes:

- Brownian Motion
- Vertical Sedimentation (Settling), radial Drift
- Turbulence in the Disk



(J.Blum)

Particles have relative velocity with gas \Rightarrow Drag forces Problems: 1) Destructive collisions, 2) Bouncing collisions, 3) fast Drift so called meter-sized barrier

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Context Growth Principle I



- Van der Waals
- Sticking enhancement with ice
- Organic compounds

Context Growth Principle II

Two basic growth modes:

BPCA

Ballistic Particle-Cluster Agglomeration: Connect individual particles



(A. Seizinger)

Example with N = 1024 Particles (here 100% Sticking) Problems: Sticking probability, velocity dependence, rolling friction, Destruction in collisions, compactification, etc ...

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BCCA

Connect whole clusters

Ballistic Cluster-Cluster Agglomeration:

Initial Growth: Experimentally Context

Test of different experimental conditions (mit $v_{\rm rel} \approx 10^{-4} - 10^{-2}$ m/s)



Wurm & Blum 1998

Differential sedimentation



Blum et al. 1998

Brownian motion



Blum et al. 2000

100 **Fractal** Growth Mass (m)-Size (s) Relation: <u>m</u>(t) / m₀ $m \propto s^{D_f}$ mit $D_f \leq 2$ 10 Typical here: $1.4 \le D_f \le 1.8$ $m(t) \propto t^{1.7}$ Approximative: 0.1



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- Assume Dust Aggregates consist of individual monomers
- Take equal sized, spherical monomers
- Need interaction model
- Not simple non-interaction billard balls
- local attractive force
- force depends on history
- use specific physical model
- Integration: Discrete Element Method
- Molecular dynamics type

Model the motion of N Particles with Newtonian Dynamics



Each spherical grain is described by the following properties

m	mass
Ι	moment of inertia
r	radius
\vec{x}	position
\vec{v}	velocity
$ec{\omega}$	angular velocity
\vec{F}	force acting on particle
\vec{M}	torque acting on particle

Plus additional **material** parameter Young's modulus (E): tensile stress divided by strain Poisson's ratio (ν): ratio transverse to axial strain Shear modulus (G): shear stress divided by strain Surface energy (γ): per unit contact area

Two *freely moving* particles **form a contact** if

$$\|\vec{x}_i - \vec{x}_j\| \le r_i + r_j$$



On impact, some of the material the particles are made of forms a circular **contact area**.

Some of the kinetic energy is dissipated (Chokshi et al. 1993). **No longrange force**: Particles must be in contact to interact with each other. Each particle can be part of several contacts.



Use **contact pointers** to describe the geometry (Dominik & Nübold, 2002).

In stress free equilibrium they are the normal vectors of the contact area.

The interaction may be divided into the following types:

- a) Compression/Adhesion (Johnson *et al.*, 1971)
- b) Rolling (Dominik & Tielens, 1995)
- c) Sliding (Dominik & Tielens, 1996)



d) Twisting

(Dominik & Tielens, 1996)

Forces and torques of those types of interaction can be derived from *corresponding potentials* (Wada *et al.*, 2007) Advantage: Can track in detail the energy evolution. We define the compression length $\delta := r_i + r_j - \|\vec{x}_i - \vec{x}_j\|$



 $\delta > 0$

 $\delta < 0$

An established contact will break if $-\delta$ exceeds the critical compression length δ_c .

Note the sign convention of δ .



FIG. 1.—Contact geometry: Two grains make contact over a finite circular area with radius *a*. The size of the area is controlled by the competition between attractive (van der Waals, dipole, etc.) forces and repulsive elastic forces.

The contact area is given by: πa^2 , where a is the contact radius.

4 dissipation Channels in contact dynamics of micron-sized particles (from: Dominik & Tielens, 1997)



- a) neck formation during pull-off
- b) lagging of contact area during rolling
- c) surface roughness
- d) jump-wise sliding of individual atoms



FIG. 2.—Schematic of the deformation during the collision process. At contact, a finite contact area is rapidly formed. This contact area grows in size during the compression and slowing down of the collision partners. Upon reversal of the collision process, the two grains will pull out a neck area, until they separate at a critical displacement, δ_c . See text for details.

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- Based on JKR-Theory (Johnson, Kendall, Roberts, 1971)
- Establishing or breaking contacts dissipates kinetic energy (Chokshi *et al.* 1993)
- Additional damping of normal oscillations (Paszun & Dominik 2008)



According to JKR-Theory (Johnson et al. 1971), the force acting on two particles that are in contact is given by

$$\frac{F}{F_c} = 4\left(\frac{a}{a_0}\right)^3 - 4\left(\frac{a}{a_0}\right)^{\frac{3}{2}}$$

where a denotes the radius of the contact area. We can obtain a via

$$\frac{\delta}{\delta_0} = 3\left(\frac{a}{a_0}\right)^2 - 2\left(\frac{a}{a_0}\right)^{\frac{1}{2}}$$

The potential energy linked with this force is given by

$$\frac{U_{normal}}{F_c \delta_c} = 6^{\frac{1}{3}} \left[\frac{16}{5} \left(\frac{a}{a_0} \right)^5 - \frac{16}{3} \left(\frac{a}{a_0} \right)^{\frac{7}{2}} + \frac{4}{3} \left(\frac{a}{a_0} \right)^2 \right]$$

(F_c =Pulloff-Force, δ_0 , a_0 equilibrium values)

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Two particles that are rolling over each other satisfy

$$\|x_i - x_j\| = const$$

However the contact area has to follow, which causes a torque that counteracts the rolling motion.



The rolling displacement $\vec{\xi}$ is defined as

$$\vec{\xi} := R(\vec{n}_1 + \vec{n}_2)$$

From the rolling potential U_r (Wada *et al.* 2007)

$$U_r = \frac{1}{2}k_r \|\vec{\xi}\|^2$$

we obtain the torques

$$\vec{M}_{r,12} = -\vec{n}_1 \times \nabla_{n_2} U_r = k_r R^2 \vec{n}_2 \times \vec{n}_1$$

which satisfy $\vec{M}_{r,12} + \vec{M}_{r,21} = 0$ $1/R = 1/r_1 + 1/r_2$ (*R*: reduced radius)



The sliding displacement is defined

$$\vec{\zeta} := r \left(\vec{n}_1 - \vec{n}_2 - \langle \vec{n}_1 - \vec{n}_2, \vec{n}_c \rangle \cdot \vec{n}_c \right)$$

Sliding

Again, the sliding potential is given by

$$U_s = \frac{1}{2}k_s \|\vec{\zeta}\|^2$$

The result is both a force and a torque counteracting the sliding motion.



Twisting describes the rotation of particles around the axis normal to the contact area.

$$\vec{\Phi} := \vec{n}_c \int_{t_0}^t \left(\vec{\omega}_i - \vec{\omega}_j \right) \cdot \vec{n}_c \, dt$$

From the twisting potential

$$U_t := \frac{1}{2} k_t \|\vec{\Phi}\|^2$$

we derive the torques caused by twisting

$$\vec{M}_{i,t} = -k_t \vec{\Phi}$$
$$\vec{M}_{j,t} = k_t \vec{\Phi}$$



- We use *contact pointers* (Dominik & Nübold, 2002) to track the time evolution of the contact area
- If certain limits are exceeded, the particle motion enters the inelastic regime
- This is reflected by modifications of the contact pointers
- The change of the potential energy due to these modifications can be tracked



Elastic motion only for small displacements. If displacement exceeds a critical value

 $\|\xi\| > \xi_{crit}$

modify contact pointers

$$\vec{n}_i \longrightarrow \vec{n}_i^c$$

 $\vec{n}_j \longrightarrow \vec{n}_j^c$

in such a way that

$$\left|\xi^{c}\right\| = \xi_{crit}$$

Energy dissipation due to this modification can be written as

$$\Delta E = k_r \xi_{crit} (\xi - \xi_{crit})$$

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Particle Interaction Particle Wall Interaction

- Boundary conditions have been implemented via walls, that restrict the motion of the particles.
- Forces exerted on a wall by the particles are ignored (⇒ *fixed* wall)

Particle-Wall Interaction:

 \Rightarrow derive forces/torques in the limit

of $r_1 = r_{\text{particle}}, r_2 \to \infty$

 \Rightarrow elastic and inelastic interaction

has been implemented



- The positions and velocities of the monomers have to be followed
- The rotation angle and rotational velocity have to be followed
- The orientation of the rotation axis has to be followed
- The number of contacts have to followed
- Check for exceeding critical amplitudes (normal, rolling, twisting)

The equations of motions are integrated using a second order (symplectic) method.

This Velocity-Verlet or Leapfrog scheme requires one force evaluation per time step

It can be written as a predictor-corrector scheme.

The 3D vector $\vec{n} = (n_x, n_y, n_z)$ can be rotated using the 3 Euler angles. These are not useful due to possible singularities. In numerical simulatins it is better to use the so called Euler parameter e_0, \vec{e} . Given a rotation of an angle φ around an axis \vec{u} with $||\vec{u}|| = 1$ we define

$$e_0 = \cos\left(\frac{\varphi}{2}\right)$$
 , (2)
 $\vec{e} = \hat{u}\sin\left(\frac{\varphi}{2}\right)$ (3)

These parameters satisfy

$$e_0^2 + e_1^2 + e_2^2 + e_3^2 = 1 \quad . \tag{4}$$

The motion of a contact pointer is then described by

$$\vec{n}(t) = A(t)\vec{n}_i \tag{5}$$

where the matrix A is calculated from (Goldstein, 1950)

$$A = \begin{pmatrix} e_0^2 + e_1^2 - \frac{1}{2} & e_1 e_2 - e_3 e_0 & e_1 e_3 + e_2 e_0 \\ e_1 e_2 + e_3 e_0 & e_0^2 + e_2^2 - \frac{1}{2} & e_2 e_3 - e_1 e_0 \\ e_1 e_3 - e_2 e_0 & e_2 e_3 + e_1 e_0 & e_0^2 + e_3^2 - \frac{1}{2} \end{pmatrix}$$
(6)

and the equations of motion are

$$\dot{e_0}(\vec{\omega}, \vec{e}) = -\frac{1}{2} \vec{e} \cdot \vec{\omega}$$

$$\dot{\vec{e}}(\vec{\omega}, \vec{e}) = \frac{1}{2} (e_0 \vec{\omega} - \vec{e} \times \vec{\omega})$$
(8)

(see Dominik & Nübold, 2002 or Wada ea. 2007)

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Integration

P

We must solve the following equations for each particle *i*:

$$\begin{split} \ddot{\vec{x}}_i &= \frac{\vec{F}_i}{m} & \dot{\vec{e}}_{0,i} &= -\frac{1}{2}\vec{\omega}_i \cdot \vec{e}_i \\ \dot{\vec{\omega}}_i &= \frac{\vec{M}_i}{I} & \dot{\vec{e}}_i &= \frac{1}{2}\left(e_{0,i}\vec{\omega}_i - \vec{e}_i \times \vec{\omega}_i\right) \end{split}$$

for the dynamics

for each contact

where (e_0, \vec{e}) denotes the quaternion used to represent the rotation of the particle

In the prediction step the new positions \vec{x}^{n+1} and the new rotational states e^{n+1} of the particles are calculated based on the current velocity, forces and torques.

$$\vec{x}_i^{n+1} = \vec{x}_i^n + \Delta t \ \vec{v}_i^n + \frac{\Delta t^2}{2m} \ \vec{F}_i^n$$
$$e^{n+1} = e^n + \Delta t \dot{e}^n + \frac{\Delta t^2}{2} \ddot{e}^n$$

with $e = (e_0, \vec{e})$.

At first, the new positions \vec{x}^{n+1} are used to check for newly established or broken contacts. If contacts have changed, keep track of the energy dissipated by discontinuities in the various potentials.

Afterwards we go through the list of contacts to calculate the new forces and torques.

$$\vec{F}_i^{n+1} = \sum_j \vec{F}_{ij}(\vec{x}^{n+1}, e^{n+1})$$
$$\vec{M}_i^{n+1} = \sum_j \vec{M}_{ij}(\vec{x}^{n+1}, e^{n+1})$$

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Integration Correction

Finally both the velocity v and angular velocity ω are updated using the old and new forces/torques.

$$\vec{v}_{i}^{n+1} = \vec{v}_{i}^{n} + \frac{\Delta t}{2m} \left(\vec{F}_{i}^{n} + \vec{F}_{i}^{n+1} \right)$$
$$\vec{\omega}_{i}^{n+1} = \vec{\omega}_{i}^{n} + \frac{\Delta t}{2I} \left(\vec{M}_{i}^{n} + \vec{M}_{i}^{n+1} \right)$$

Updating the particle interaction is the most expensive part:

- Search for next neighbours
- Check for breaking or formation of contacts
- For each contact: Calculate current displacements and apply possible inelastic corrections
- For every particle: Calculate current force/torque

Difficult to implement on GPUs due to irregular memory access patterns and possible data hazards.

Spatial Subdivision:

Search for next neighbours in $O(N \log(N))$

GPU Version:

Efficient implementation described by Green (2008)



- Normal vibrations (steep JKR-potential) severely limit timestep Δt , for $1.2\mu m$ SiO₂ particles $\Delta t \approx 0.2 0.4$ ns
- Due to the short timesteps the range of values is high \Rightarrow double-precision floating point arithmetics are mandatory
- Discontinuities in forces when contacts are made or breaking up



Main differences between CPU and GPU (taken from NVIDIA CUDA programming guide 2.2.1)

ALU: Arithmetic and Logical Unit

A

Compute Unified Device Architecture:

- Parallel computing architecture developed by NVIDIA
- SIMD (single instruction multiple data)
- Code targeting the GPU is written in a C-like language (CUDA C) and later linked with the serial code running on the CPU

Serial code	Host	
Parallel kernel	Device	
Kernel0<<<>>>()	Grid O	
	Block (0, 0) Block (1, 0) Block (2, 0) Image: State of the state of	
Serial code	Host	
	Device	
<pre>Parallel kernel Kernel1<<<>>>()</pre>	Grid 1	
↓	Block (0, 0) Block (1, 0)	

Alternative Theory

JKR:

(Johnson, Kendall and Roberts)

- Short-range surface forces within contact area
- $F_c = 3\pi\gamma R$
- $\delta_c > 0 \Rightarrow$ Adhesive necks
- Suitable to model larger, soft grains

DMT:

(Derjaguin, Muller and Toporov)

- Long-range surface forces outside contact area
- $F_c = 4\pi\gamma R$
- $\delta_c = 0 \Rightarrow \text{No necks}$
- Suitable to model small, hard grains

JKR and DMT model are limits of a single theory (Tabor, 1977)

JKR vs. DMT



Dust Dynamics



Material Parameter





Material properties play very important role: - Calibration with experiments required

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Experimental Dust Growth



(J. Blum, Braunschweig)

in Vacuum, zero gravity

- in lab
- fall Tower (Bremen)
- parabolic flights
- space station

initial Fractal Growth works up to cm-sizes



- Filling factor ϕ : Mean density ρ of the aggregate devided by the matrix density (of each monomer), $\phi = \rho / \rho_{\text{matrix}}$
- Porosity Φ : The complement of the filling factor, $\Phi = 1 - \phi$
- Coordination number n_c : Mean number of contacts each monomer has

Expectation: The material properties scale with the porosity

Material Parameter

Quasi-static Compression I

Dustcake between two Plates \Rightarrow Move them slowly towards each other measure force/pressure (here: Simulation by Dominik Paszun, Amsterdam)



Fig. 3. The setup of the experiment. The dust cake in the center is compressed with different pressure. Initial arrangement (a), results of compression at $2 \cdot 10^2$ Pa (b), $2 \cdot 10^3$ Pa (c), $5 \cdot 10^3$ Pa (d), $1 \cdot 10^4$ Pa (e).

Experiments in Braunschweig, Simulations Amsterdam/Tübingen

- initial filling factor: $\phi_0 = 0.15$
- radius of sphere: 0.75μ m
- Particle number: N = 291

Right: Comparison with expt. (Blum&Schräpler, 2004) (Paszun&Dominik, 2008)



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Quasi-static Compression II

a) Multi-directional compression



b) Uni-directional compression

Experimental Setup & Results

(Güttler ea. 2009)



Numerical Results (case a)

(Seizinger ea. 2012)



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Dynamic Compression

Velocity Dependence





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Material Parameter

Tensile and Shear-strength

Setups for measuring tensile and shear strength as a function of the filling factor (Seizinger ea. 2013) (Difficult to measure experimentally)

No wall glue



Measure shear strength



With wall glue



Comparison with SPH values



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Collisions Sample Generation Methods I



Collisions Particle Generation Methods II

Relation between filling factor ϕ and the coordination number n_c



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Collisions Bouncing Behaviour I

Collisions between particles with 60 $\mu \rm m$ diameter Shown is the growthfactor

$$\gamma = \frac{m_{\text{largest}}}{m_{\text{tot}}}$$

CPE aggregate





Green: Sticking Yellow: Bouncing (or onset to fragmentation) Red: Fragmentation (above \approx 10 m/s)

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Copenhagen: 23. August, 2013

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Collisions Bouncing Behaviour II

Monitor energies during the collisions (advantage of potential formulation) use here two particles (CPE and BAM) **both** with $d = 60 \mu$ m, and $\phi = 0.59$



Sticking properties depend on preparation method, i.e. not only ϕ but also n_c But: Experimentally n_c not known, only ϕ Red: Fragmentation (above \approx 10 m/s)

Collisions Bouncing/Fragmentation

Collide two CPE (Close Packing with Extraction) aggregates with coordination number $n_c = 8.11$ and filling factor $\phi = 0.52$ Two collision velocities

 $v_{\rm rel} = 2$ m/s



 $v_{\rm rel} = 5$ m/s



Collisions

Expt.: Cluster-Cluster Collisions

Sticking



Bouncing



Material:Silicate (mono- / polydispers)Size: $\approx mm - cm$ $v_{\rm Kollision}$ $\approx 0.1 - 100 \, {\rm cm/s}$

in multiple collisions: Compactification $D_f \rightarrow 3$ (S. Kothe, R. Weidling, D. Heißelmann & J. Blum, TU Braunschweig)

Collisions

Numerical: Cluster-Cluster Collisions

Initial Growth Phase



Collision with different speeds



Animations by Alexander Seizinger (Tübingen)

Larger BodiesContinuum Approach

- For larger bodies the ab initio approach is not feasible
- Perform continuum simulations
- need again material parameter

Larger Bodies

For larger particles: Our Method: SPH (Smoothed-Particle-Hydrodynamics) Hydrodynamical-Equations augmented with: Elasto-plastic Model (A-B) Including:

Fractures (C)

Example: Impact into Al-Plate (Rabczuk, 2002)



SPH Simulation: Finite Element Simulation:

Two colliding rubber rings





(Christoph Schäfer, Univ. Tübingen, 2005)



plastic Material

Investigate the growth of particles through Collisions/Accretion

2 Basalt spheres: $\rho = 3g/cm^3$, R₁=9m, R₂=7.5m, V_{rel}=25m/s , t_{max} = 4.5 sec





(Christoph Schäfer, PhD-Thesis, Univ. Tübingen 2005)

Problem : Destructive Collisions

so called *meter-sized barrier*

Possible Solution: Porous material, need Calibration simulation

Larger Bodies

Test: Dynamical Impact

Glass sphere 1 mm-diameter \Rightarrow onto dust cake



Expts.: in Braunschweig Simulations: in Tübingen

Determine:

- Braking Curve (see right plot)
- Intrusion depth
- density distribution
- Porosity



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Dust-Particle against Wall



(Ralf Geretshauser, Univ. Tübingen, 2007/08)

Glass sphere into Dust Cake



Larger Bodies

Experiment (color coded: filling factor) (M. Krause, Braunschweig)



SPH-Simulations (density)(Ralf Geretshauser& Roland Speith, Tü)



(DFG-Research Group: "First Phase of Planet Formation", 2007-2013) Joint Project: Braunschweig, Duisburg, Heidelberg & Tübingen

Idea:

Continuum Simulations of Particle Collisions determine boundary: Sticking, Bouncing, Fragmentation, catalogue as a function of relative velocity and particle size

Catastrophic Disruption Threshold: (that specific energy *Q*, at which the largest intact particle has = 1/2 Targetmass) Collisions of Basalt spheres



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Check growth of planetesimals by collisions/accretion

SPH (Smoothed-Particle-Hydrodynamics) using 250,000-500,000 particles Here: Elastic-plastic strength model, formation and evolution of cracks

2 Basalt Spheres:





(cp. small objects in Solar System)

(Schäfer, Geretshauser, Speith, Meru; Tübingen) (Geretshauser ea., 2010, 2011a,b)

 \Rightarrow Need porous bodies !

Larger Bodies

Growth Regime



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Initial planetary growth through collisions of dust agregates

- Modelling by molecular dynamics
- 4 types of motion (normal, rolling, sliding, twisting)
- Non-elastic energy dissipation
- Computing on GPUs
- Determine continuum parameter

For larger particles

- Continuum SPH simulations
- Determine Fragmentation Threshold

Dust Dynamics The End

