To Be Planetesimals, or Not to Be: That is the Question of Dust Aggregates.

Numerical Simulations of Dust Aggregate Collisions

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Collisional growth of dust ($< \mu m$) → Planetesimal formation ($> km$) → Numerical simulation of dust aggregate collisions!

Structure evolution of dust aggregates in protoplanetary disks:

- When and how are aggregates compressed and/or disrupted?
- Can dust aggregates grow through collisions?
Grain interaction model

Elastic spheres having surface energy

Normal Sliding rolling twisting

Contact & Separation

$s, \xi, \phi > \text{critical displacements}$

Energy dissipation

- Critical slide
  $s_{crit} \sim 1.5 \text{ Å} \quad \text{(for 0.2 µm quartz)}$
- Critical roll
  $\xi_{crit} \sim 2 \text{ Å} \quad \text{(or} \sim 30 \text{ Å (Heim et al., 1999))}$
- Critical twist
  $\phi_{crit} \sim 1^\circ$

$E_{break}$: Energy to break a contact
$E_{roll}$: Energy to roll a pair of grains by $90^\circ$

References:
Johnson, Kendall and Roberts (1971)
Johnson (1987), Chokshi et al. (1993)
Dominik and Tielens (1995, 96)
Wada et al. (2007)
Today’s topics

Can dust grow through collisions?

for Low-velocity collisions
○ Does “bouncing barrier” for dust growth really exist? No!

for high-velocity collisions
○ Do collisions between different-sized aggregate encourage dust growth? Partly Yes.
Bouncing Conditions

*To bounce, or not to bounce?*
Bouncing Problem

“Bouncing” prevents dust from growing

Previous numerical simulations:
Dominik & Tielens 1997;
Wada et al. 2007, 2008, 2009;
Suyama et al. 2008, etc…

No bouncing  ➡️  Collisional growth is feasible!

\[ BPCA, N=8000+8000, \text{ ice, } \xi_c = 8\text{Å}, u_{col} = 70 \text{ m/s} \ (E_{imp} = 42 \text{ NE}_{break}) \]
Fig. 5. Examples for the experimental outcomes in the collisions of small aggregates with a solid target. The collision can lead to sticking, bouncing, or fragmentation (from left to right). The time between two exposures is 2 ms.

\[ u_{\text{col}} \approx 1 \text{ m/s} \]

Bouncing in experiments

\[ \text{Sticking} \quad \rightarrow \quad \text{Bouncing} \quad \rightarrow \quad \text{Fragmentation and/or sticking} \]
Bouncing condition

- Why bouncing in experiments?
- What’s the condition for bouncing?

Hypothesis: Number of contacts controls?

Bouncing would be caused by immobility of particles, inhibiting energy dissipation.

Aggregates in numerical simulations:
Number of particles in contact with a particle (Coordination number, C.N.) = 2~4, on average

More C.N. in experiments?
Objective

- To reveal the dependence on coordination number for aggregate bouncing

Simulation of aggregate collisions

Parameter: Coordination Number (C.N.)

Idea for making required C.N.:

Extracing particles randomly
from close-packed structure (C.N.=12)

aggregates with C.N. = ~12 to ~3
Initial conditions and settings

✓ (hexagonal) close-packed aggregates:
  mean C.N. ~ 11
  - Number of particles: 4197 (3 types randomly produced)

✓ particle-extracted aggregates:
  extraction rate \( f = 0.05 - 0.75 \)  C.N. ~ 12 \((1 - f)\)

- \( f = 0.2 \)
  mean C.N. = 8.8

- \( f = 0.5 \)
  mean C.N. = 5.5

- \( f = 0.75 \)
  mean C.N. = 2.8

✓ Ice \((E = 7.0 \text{ GPa}, \nu = 0.25, \gamma = 100 \text{ mJ/m}^2, R = 0.1 \mu\text{m})\), critical rolling displace. \( \xi_{\text{crit}} = 8\AA \)

✓ SiO\(_2\) \((E = 54 \text{ GPa}, \nu = 0.17, \gamma = 25 \text{ mJ/m}^2, R = 0.1 \mu\text{m})\), critical rolling displace. \( \xi_{\text{crit}} = 8\AA \)

✓ \( u_{\text{col}} = 0.1 - 22 \text{ m/s} \) (Ice), 0.01 - 2.2 m/s (SiO\(_2\))
Examples of simulation (Ice)

C.N. = 11

\[ u_{\text{col}} = 0.096 \text{ m/s} \quad (E_{\text{imp}} = 0.66 \ E_{\text{break}}) \]

C.N. = 8.8

\[ u_{\text{col}} = 0.096 \text{ m/s} \quad (E_{\text{imp}} = 0.53 \ E_{\text{break}}) \]

C.N. = 5.5

\[ u_{\text{col}} = 0.38 \text{ m/s} \quad (E_{\text{imp}} = 5.3 \ E_{\text{break}}) \]

C.N. = 2.8

\[ u_{\text{col}} = 0.38 \text{ m/s} \quad (E_{\text{imp}} = 2.7 \ E_{\text{break}}) \]
Examples of simulation (Ice)

C.N. = 11

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C.N. = 2.8

\[ u_{\text{col}} = 0.38 \text{ m/s} \quad (E_{\text{imp}} = 2.7 E_{\text{break}}) \]
Examples of simulation (Ice)

C.N. = 11

\[ u_{\text{col}} = 1.5 \, \text{m/s} \quad (E_{\text{imp}} = 170 \, E_{\text{break}}) \]

C.N. = 8.8

\[ u_{\text{col}} = 1.5 \, \text{m/s} \quad (E_{\text{imp}} = 135 \, E_{\text{break}}) \]

C.N. = 5.5

\[ u_{\text{col}} = 1.5 \, \text{m/s} \quad (E_{\text{imp}} = 85 \, E_{\text{break}}) \]

C.N. = 2.8

\[ u_{\text{col}} = 1.5 \, \text{m/s} \quad (E_{\text{imp}} = 43 \, E_{\text{break}}) \]
Examples of simulation (Ice)

C.N. = 11

\[ u_{\text{col}} = 1.5 \text{ m/s } (E_{\text{imp}} = 170 E_{\text{break}}) \]

C.N. = 8.8

\[ u_{\text{col}} = 1.5 \text{ m/s } (E_{\text{imp}} = 135 E_{\text{break}}) \]

C.N. = 5.5

\[ u_{\text{col}} = 1.5 \text{ m/s } (E_{\text{imp}} = 85 E_{\text{break}}) \]

C.N. = 2.8

\[ u_{\text{col}} = 1.5 \text{ m/s } (E_{\text{imp}} = 43 E_{\text{break}}) \]
Examples of simulation (Ice)

C.N. = 11

\[ u_{\text{col}} = 22 \text{ m/s} \quad (E_{\text{imp}} = 4.1 \times N E_{\text{break}}) \]

C.N. = 8.8

\[ u_{\text{col}} = 22 \text{ m/s} \quad (E_{\text{imp}} = 4.1 \times N E_{\text{break}}) \]

C.N. = 5.5

\[ u_{\text{col}} = 22 \text{ m/s} \quad (E_{\text{imp}} = 4.1 \times N E_{\text{break}}) \]

C.N. = 2.8

\[ u_{\text{col}} = 22 \text{ m/s} \quad (E_{\text{imp}} = 4.1 \times N E_{\text{break}}) \]
Examples of simulation (Ice)

C.N. = 11

\[ u_{\text{col}} = 22 \text{ m/s} \ (E_{\text{imp}} = 4.1 \ N \ E_{\text{break}}) \]

C.N. = 8.8

\[ u_{\text{col}} = 22 \text{ m/s} \ (E_{\text{imp}} = 4.1 \ N \ E_{\text{break}}) \]

C.N. = 5.5

\[ u_{\text{col}} = 22 \text{ m/s} \ (E_{\text{imp}} = 4.1 \ N \ E_{\text{break}}) \]

C.N. = 2.8

\[ u_{\text{col}} = 22 \text{ m/s} \ (E_{\text{imp}} = 4.1 \ N \ E_{\text{break}}) \]
Result: Bouncing Condition (Ice)

Collision velocity [m/s]

Mean Coordination Number

- Bouncing
- Mean C.N. < ~ 6
- Sticking

$E_{\text{impact}} / (N E_{\text{break}})$
Result: Bouncing Condition (SiO₂)

Mean Coordination Number vs. Collision velocity [m/s]

- Bouncing
- Mean C.N. < ~ 6
- Sticking

Graph showing the relationship between mean coordination number and collision velocity for different impact energies normalized by the energy of break.
Result: Bouncing Condition (Ice, SiO$_2$)

No difference between Ice and SiO$_2$

Scaled well by using $E_{\text{break}}$
Why C.N. = 6 ?

A particle cannot move freely with C.N. = 6 in 3D:
C.N.@BPCA collisions

Ice, 8Å, 8000+8000

Mean Coordination Number

\[ E_{\text{impact}} / (N E_{\text{break}}) \]

\[ u_{\text{col}} \text{ [m/s]} \]

Legend:
- \( b = 0.00 \) (red)
- \( b = 0.19 \) (green)
- \( b = 0.39 \) (blue)
- \( b = 0.49 \) (magenta)
- \( b = 0.58 \) (cyan)
- \( b = 0.69 \) (yellow)
- \( b = 0.78 \) (black)
- \( b = 0.89 \) (red)
- \( b = 1.00 \) (gray)
- Average (black)
Why C.N. = 4?

A particle cannot move freely with C.N. = 6 in 3D:

But, stable enough with at least C.N. = 4 in 3D:
aggregates produced by collisions

BPCA, \( N=8000+8000 \), ice, \( \xi_c = 8\text{Å} \), \( u_{\text{col}} = 57 \text{ m/s} \) \( (E_{\text{imp}} = 27 \text{ NE}_{\text{break}}) \)

Initial condition (C.N. = 3.8)

15288+15288
Collisions of collision-produced aggregates (C.N. = 3.8)

$u_{\text{col}} = 0.38 \text{ m/s} \ (E_{\text{imp}} = 1.2 \times 10^{-3} \text{ NE}_{\text{break}})$

$u_{\text{col}} = 0.77 \text{ m/s} \ (E_{\text{imp}} = 5.1 \times 10^{-3} \text{ NE}_{\text{break}})$

$u_{\text{col}} = 1.54 \text{ m/s} \ (E_{\text{imp}} = 2.0 \times 10^{-2} \text{ NE}_{\text{break}})$

$u_{\text{col}} = 17.4 \text{ m/s} \ (E_{\text{imp}} = 2.6 \text{ NE}_{\text{break}})$
Structure is also important?

C.N. = 6
Cubic lattice

C.N. = 2.35

C.N. = 6  BAM-2

C.N. = 4  BAM-1

Ballistic Agglomeration with Migration (BAM)

Shen, Draine, and Johnson (2008)
Structure is not important.

C.N. = 6

C.N. = 2.35

C.N. = 6

C.N. = 4

No!
Bouncing only for C.N. \( \approx 6 \)
Summary

We examine the bouncing condition, focusing on C.N. of aggregates.

- Always sticking if C.N. < 6.
- Collision velocity for transition from bouncing to sticking is consistent with experimental results.
- Collision-produced aggregates have C.N. < 4

Not to bounce.

It is feasible to form planetesimals through direct collisions of dust aggregates.

C.N. ~ 2 for aggregates in experiments?

FIG. 2 (color online). (a) An example of an agglomerate with a volume filling factor of 0.15. (b) Specimen of an agglomerate after manual cutting to 10 x 10 mm². (c) Result of a Monte Carlo simulation of ballistic deposition. (d) High resolution scanning electron microscopy (SEM) image of the surface of an agglomerate consisting of SiO2 spheres with 1.5 m diameter.

(Blum & Schräpler 2004)
A Hard Shell?

\[ \frac{a}{b} = 0.8 \]

\[ u_{\text{col}} = 1.1 \text{ m/s (vimp = 3)} \]

\( f = 0.75 \)
mean C.N. = 2.8

\( f = 0.2 \)
mean C.N. = 8.8

Ice
Collisions between different-sized dust aggregates
Ballistic Particle-Cluster Aggregation (BPCA)

- Formed by one-by-one sticking of monomers

- Compact structure (fractal dimension ~ 3)

Dust is expected to be compact at high velocity collisions causing their disruption

Collisions of BPCA clusters → implication for growth and disruption of dust
Motivation

Collision velocity of dust in protoplanetary disks

< several 10 m/s!

e.g., < \sim 50 m/s (Hayashi model, without turbulence)

Is it possible for dust to grow through collisions?

Possible for ice dust of equal-sized aggregates

\( u_{\text{coll}} \) for silicate = 0.1 \times \( u_{\text{coll}} \) for ice

But, for silicate dust?

What if different-sized?

Objective

Do collisions of different-sized aggregates encourage dust growth?

Simulations of collisions between

**BPCAs** of different sizes

✓ Growth efficiency: \( f = \frac{(N_{\text{large}} - N_{\text{target}})}{N_{\text{proj}}} \)

Size dependence

Size-ratio dependence
Initial Conditions and Parameters

Collisions of BPCA clusters: projectile vs. target

- **Size ratio** = 1 : 16 (2000:32000, 8000:128000)
- 1 : 64 (500:32000, 2000:128000, 8000:512000)

- **Impact parameter**: $b$ (defined by using characteristic radius)

- **Ice** ($E = 7.0 \times 10^{10}$ Pa, $\nu = 0.25$, $\gamma = 100$ mJ/m$^2$, $R = 0.1\mu$m), critical rolling displacement $\xi_{\text{crit}} = 8\text{Å}$

- **Collision velocity** $u_{\text{coll}} = 15 - 300$ m/s
Examples of simulations

$2000 : 128000 \ (= 1 : 64)$ ice, $u_{\text{coll}} = 52 \text{ m/s}$

$b = 0$

$b = 0.69$

effectively captured

$8000 : 8000$

$8000 : 8000$

$b = 0$

$b = 0.69$
Growth efficiency (ice)

\[ f \equiv \frac{N_{\text{large}} - N_{\text{target}}}{N_{\text{proj}}} \]

- \( f > 0 \) → mass gain
- \( f < 0 \) → mass loss

8000 : 8000 = 1 : 1
Growth efficiency (ice)

\[ f \equiv \frac{N_{\text{large}} - N_{\text{target}}}{N_{\text{proj}}} \]

: growth efficiency

\[ \begin{align*}
\{ \ & f > 0 \rightarrow \text{mass gain} \\
\ & f < 0 \rightarrow \text{mass loss}
\end{align*} \]

- \( 8000 : 8000 = 1 : 1 \)
- \( 2000 : 32000 = 1 : 16 \)
Growth efficiency (ice)

\[ f \equiv \frac{(N_{\text{large}} - N_{\text{target}})}{N_{\text{proj}}} \]

- \( f > 0 \) → mass gain
- \( f < 0 \) → mass loss

No size dependence

\[
\begin{align*}
8000 : 8000 &= 1 : 1 \\
2000 : 32000 &= 1 : 16 \\
8000 : 128000 &= 1 : 16
\end{align*}
\]
Growth efficiency

\( f \equiv \frac{N_{\text{large}} - N_{\text{target}}}{N_{\text{proj}}} \) : growth efficiency

\( \begin{align*}
&\text{mass gain} \\
&\text{mass loss}
\end{align*} \)
Growth efficiency (ice)

\[ f \equiv \frac{(N_{\text{large}} - N_{\text{target}})}{N_{\text{proj}}} : \text{growth efficiency} \]

\[ \begin{align*}
8000 : 8000 &= 1 : 1 \\
2000 : 32000 &= 1 : 16 \\
8000 : 128000 &= 1 : 16 \\
500 : 32000 &= 1 : 64 \\
2000 : 128000 &= 1 : 64
\end{align*} \]

\[ u_{\text{coll}} \text{ [m/s]} \]
Growth efficiency (ice)

\[ f \equiv \frac{N_{\text{large}} - N_{\text{target}}}{N_{\text{proj}}} \]

- \( f > 0 \rightarrow \) mass gain
- \( f < 0 \rightarrow \) mass loss

No size dependence

Dependent on size ratio

The larger ratio, the more gain.

No increase in the critical velocity

\(< 100 \text{ m/s}\)
Summary and Implication

Simulations of collisions of different-sized BPCAs

- Large size-ratio leads to large growth efficiency.
  - encouraging dust growth and planetesimal formation

- The critical collision velocity $u_{\text{coll,crit}}$ is unchanged.
  - $u_{\text{coll,crit}}$ for ice $< 100$ m/s
  - $u_{\text{coll,crit}}$ for silicate $= 0.1 \times u_{\text{coll,crit}}$ for ice $< 10$ m/s

- It is still difficult for silicate dust to grow?
Can dust grow through collisions?

**Take-home messages**

**for Low-velocity collisions**
- Does “bouncing barrier” for dust growth really exist?  
  → No!

**for high-velocity collisions**
- Do collisions between different-sized aggregate encourage dust growth?  
  → Partly Yes,  
  But, not enough for silicate dust.
Collisions of BPCA clusters

- BPCA clusters are:
  - composed of 500, 2000, or 8000 particles (3 types randomly produced)
  - Impact parameter: \( b \) (defined by using characteristic radius \( r_c \))

\[
b = \frac{l}{r_{c,a} + r_{c,b}}
\]

\[
r_c = \sqrt{\frac{5}{3N} \sum (x_i - x_G)^2}
\]

- Ice \( (E = 7.0 \times 10^{10} \text{ Pa}, \nu = 0.25, \gamma = 100 \text{ mJ/m}^2, R = 0.1 \mu\text{m}) \), critical rolling displace. \( \xi_{\text{crit}} = 8 \text{Å} \)

- Impact velocity \( v_{\text{imp}} = 6 - 300 \text{ m/s} \)
Collisions of BPCA clusters

$N=8000+8000$, ice, $\xi_c = 8\text{Å}$, $v_{imp} = 70 \text{ m/s}$ ( $E_{imp} = 42 \text{ NE}_\text{break}$ )

$b = 0$

$b = 0.39$

$b = 0.69$

$b = 1.00$
Largest fragment mass $N_{\text{large}}$:

**growth efficiency**

\[ f = \frac{N_{\text{large}}}{N_{\text{total}}} \]

- $f > 0.5 \rightarrow +$ growth
- $f < 0.5 \rightarrow -$ growth

\( f \) dependent on \( N \)
Probability of collisions within \([b, b+\text{db}]\)

\[ b = \frac{l}{2r_c} \]

\[
P(b)\,db = \frac{2\pi l \, dl}{\pi (2r_c)^2} = \frac{\pi (2r_c)^2 \, 2b \, db}{\pi (2r_c)^2} = 2b \, db \quad (0 \leq b \leq 1)
\]

\[
= dB^2 \quad (0 \leq b^2 \leq 1)
\]

Average value of \(f\)

\[
f = \frac{\int_0^1 f \, db^2}{\int_0^1 db^2} = \int_0^1 f(b^2) \, db^2
\]
Growth efficiency: $f(b^2)$

$f$ as a function of $b^2$

\[ f \equiv \frac{N_{\text{large}}}{N_{\text{total}}} \]

: growth efficiency

\[
\begin{align*}
&f > 0.5 \rightarrow + \text{ growth} \\
&f < 0.5 \rightarrow - \text{ growth}
\end{align*}
\]

\[
\bar{f} = \int_{0}^{1} f(b^2) \, db^2
\]
Largest fragment mass $N_{\text{large}}$: growth efficiency

$$f = \frac{N_{\text{large}}}{N_{\text{total}}}$$

- $f > 0.5 \rightarrow +$ growth
- $f < 0.5 \rightarrow -$ growth

Average weighted by $b^2$
Growth efficiency averaged

\[ f \equiv \frac{N_{\text{large}}}{N_{\text{total}}} \]

: growth efficiency

\[ \begin{align*}
    f > 0.5 \rightarrow + \text{ growth} \\
    f < 0.5 \rightarrow - \text{ growth}
\end{align*} \]
Growth efficiency averaged

\[ \nu_{\text{imp}} \ [\text{m/s}] \ (\text{ice}) \]

\[ f = \frac{N_{\text{large}}}{N_{\text{total}}} \]

\[ f > 0.5 \rightarrow + \text{ growth} \]
\[ f < 0.5 \rightarrow - \text{ growth} \]

\(~ 60 \text{ m/s}~

small dependence on \( N \)

Averaged for \( b^2 \)
Averaged growth efficiency for BCCA clusters

\[ f = \frac{N_{\text{large}}}{N_{\text{total}}} \]

\[ v_{\text{imp}} \text{ [m/s] (ice)} \]

\[ E_{\text{impact}} / (N E_{\text{break}}) \]

\( \sim 37 \text{ m/s} \)

\( \checkmark \) independent of \( N \)

Averaged over \( b^2 \)
Averaged growth efficiency: \textit{BCCA} & \textit{BPCA}

\[ \nu_{\text{imp}} [\text{m/s}] (\text{ice}) \]

\[ f = \frac{N_{\text{large}}}{N_{\text{total}}} \]

Actual dust structure: between \textit{BCCA} and \textit{BPCA}

Averaged over $b^2$