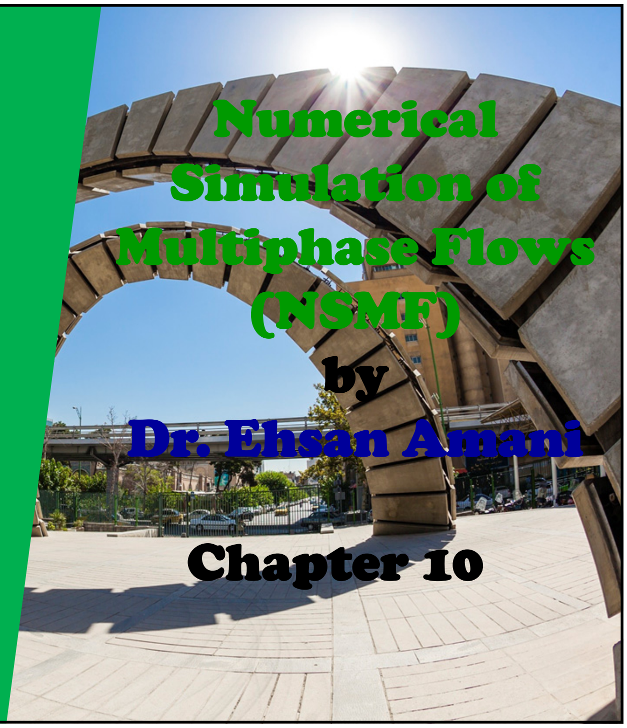


Numerical Simulation of Multiphase Flows (NSMF)

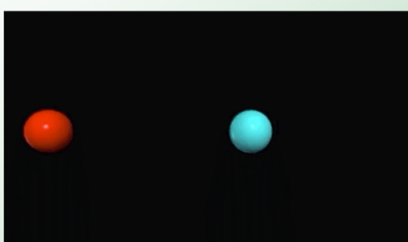
by

Dr. Ehsan Amani

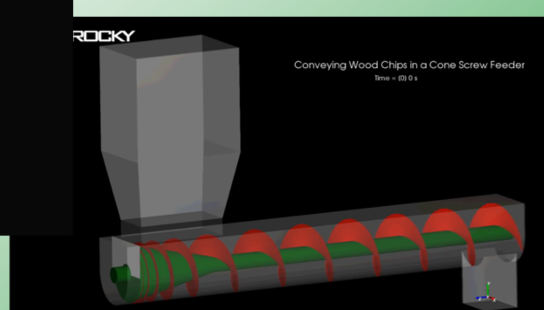
Chapter 10

Particle-particle interaction (PPI)

- PPI classification:
  - Collision and contact



▲ **Collison: short duration contact**



▲ **Contact: conveying wood chips in a cone screw feeder**

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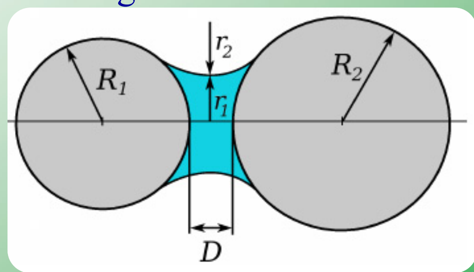
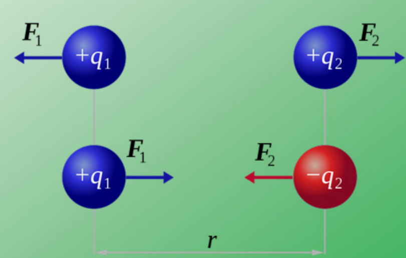
Particle-particle interaction (PPI)

- PPI classifications:
  - Collision and contact
  - Inter-particle forces: affects collision outcome or incidence
    - Liquid bridge



Particle-particle interaction (PPI)

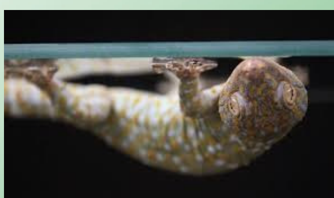
- PPI classifications:
  - Collision and contact
  - Inter-particle forces:
    - Liquid bridge
    - Electrostatic forces



$$|\boldsymbol{F}_1| = |\boldsymbol{F}_2| = k_e \frac{|q_1 \times q_2|}{r^2}$$

Particle-particle interaction (PPI)

- PPI classifications:
  - Collision and contact
  - Inter-particle forces:
    - Liquid bridge
    - Electrostatic forces
    - Van der Waals force



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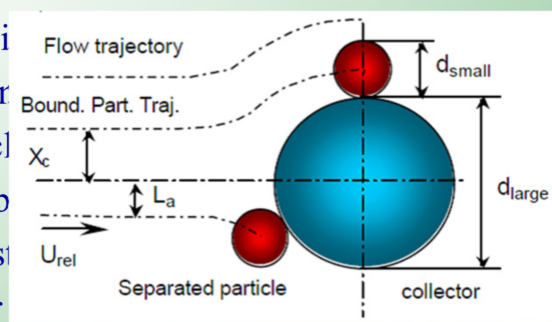
Particle-particle interaction (PPI)

- PPI classificati
  - Collision ar
  - Inter-particl
    - Liquid b
    - Electrost
    - Van der
    - Lubrication force



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Particle-particle interaction (PPI)

- PPI classifications:
  - Collision and contact
  - Inter-particle forces:
    - Liquid bridge
    - Electrostatic forces
    - Van der Waals force
    - Lubrication force
  - Other interactions …

Collision modeling approaches

- Hard-sphere
  - Binary collision
  - Dispersed regime
- Soft-sphere (discrete element method (DEM))
  - Multiple collision
  - Dense regime
  - High-computational costs
- Multiphase particle-in-cell (MP-PIC) method
- …

Lagrangian collision model stages

- Collision incidence: finding the collision pair
  - Numerically challenging
  - Uncertainties
  - Classification:
    - ✓ Deterministic
    - ✓ Stochastic
    - ✓ Hybrid

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Lagrangian collision model stages

- Collision incidence: finding the collision pair
- Collision outcome: post-collision properties
  - Bouncing
  - Coalescence
  - Agglomeration
  - Shattering
  - Reflexive/stretching separation
  - …

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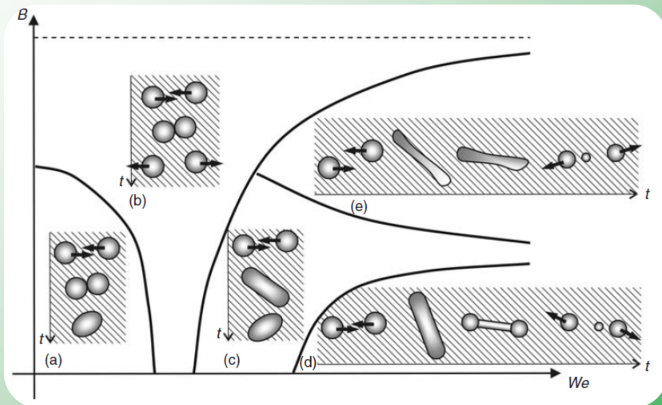
Lagrangian collision model stages

- Collision incidence: finding the collision pair
- Collision outcome: post-collision properties



◄ **Regimes of hydrocarbon drops collisions:**
(a) coalescence;
(b) bouncing;
(c) coalescence;
(d) reflexive separation;
(e) stretching separation.

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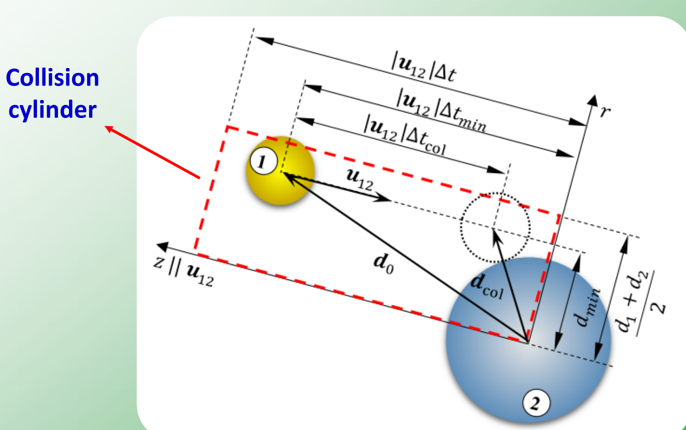
Trajectory (direct) collision model

- Collision incidence: deterministic
  - For every particle pair 1 and 2:



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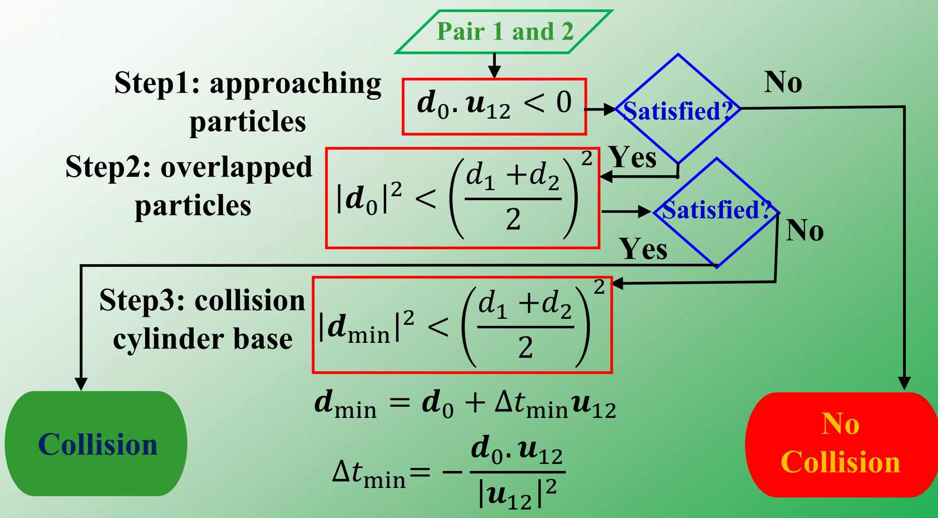
Trajectory (direct) collision model

- Collision incidence: deterministic



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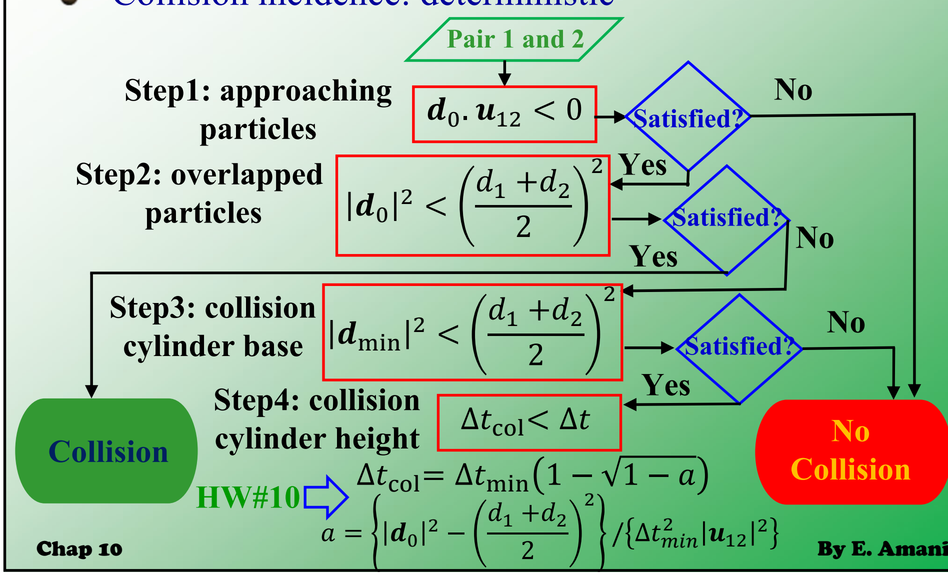
Trajectory (direct) collision model

- Collision incidence: deterministic



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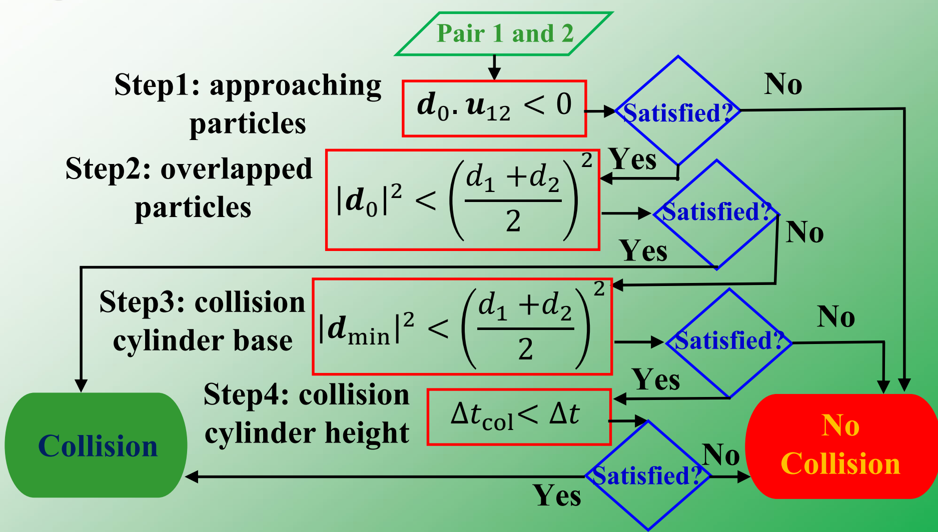
Trajectory (direct) collision model

- Collision incidence: deterministic



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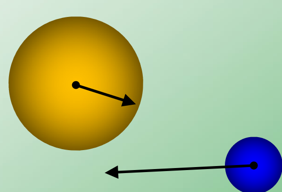
Trajectory (direct) collision model

- Collision outcome: solid particles
  - For every collision incidence:

$n \rightarrow \mathrm{col}$



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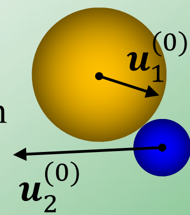
Trajectory (direct) collision model

- Collision outcome: solid particles
  - For every collision incidence:

$n \rightarrow \text{col}$

Just before
the collision



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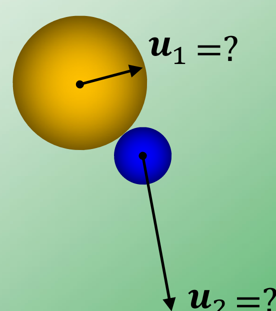
Trajectory (direct) collision model

- Collision outcome: solid particles
  - For every collision incidence:

$n \rightarrow \text{col}$

Just after
the collision



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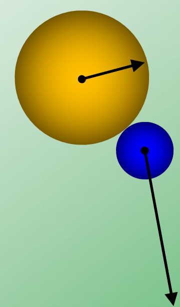
Trajectory (direct) collision model

- Collision outcome: solid particles
  - For every collision incidence:

$n \rightarrow \text{col} \rightarrow n + 1$



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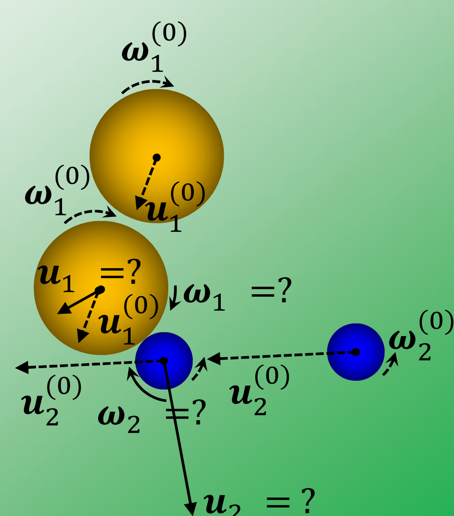
Trajectory (direct) collision model

- Calculation of important quantities just before the collision:

$$\boldsymbol{G}^0 \equiv \boldsymbol{u}_{12}^0 = \boldsymbol{u}_1^0 - \boldsymbol{u}_2^0$$



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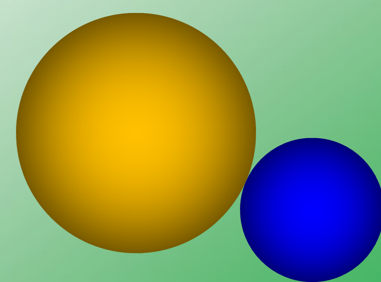
Trajectory (direct) collision model

- Calculation of important quantities just before the collision:

$$G^0 \equiv u_{12}^0 = u_1^0 - u_2^0$$



Trajectory (direct) collision model

- Calculation of important quantities just before the collision:

$$\boldsymbol{G}^0 \equiv \boldsymbol{u}_{12}^0 = \boldsymbol{u}_1^0 - \boldsymbol{u}_2^0$$

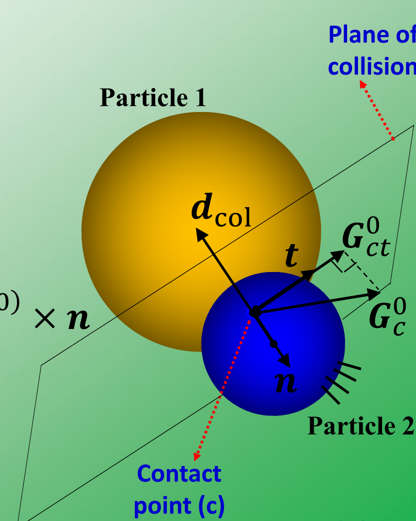
$$\boldsymbol{n} = -\frac{\boldsymbol{d}_{\text{col}}}{|\boldsymbol{d}_{\text{col}}|}$$

$$\boldsymbol{d}_{\text{col}} = \boldsymbol{d}_0 + \Delta t_{\text{col}} \boldsymbol{u}_{12}^0$$

$$\boldsymbol{G}_c^0 = \boldsymbol{G}^0 + r_1 \boldsymbol{\omega}_1^{(0)} \times \boldsymbol{n} + r_2 \boldsymbol{\omega}_2^{(0)} \times \boldsymbol{n}$$

$$\boldsymbol{G}_{ct}^0 = \boldsymbol{G}_c^0 - (\boldsymbol{G}_c^0 . \boldsymbol{n})\boldsymbol{n}$$

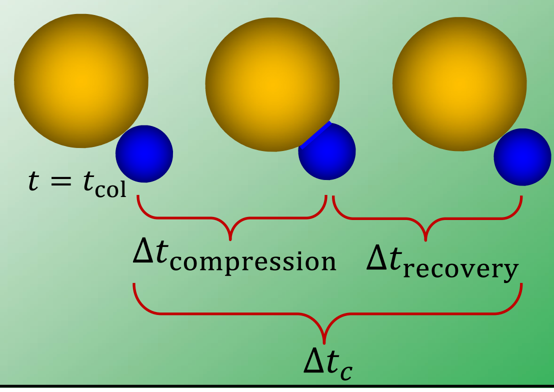
$$\boldsymbol{t} = \frac{\boldsymbol{G}_{ct}^0}{|\boldsymbol{G}_{ct}^0|}$$



Trajectory (direct) collision model

- The linear momentum equation for each particle (p = 1 or 2):

$$m_p \frac{d\boldsymbol{u}_p}{dt} = \boldsymbol{F}_{\text{col},p} + \boldsymbol{F}_{\text{other},p}$$



Trajectory (direct) collision model

- The linear momentum equation for each particle (p = 1 or 2):

$$m_p \frac{d\boldsymbol{u}_p}{dt} = \boldsymbol{F}_{\text{col},p} + \boldsymbol{F}_{\text{other},p}$$

- Integration over Δt_c, assuming
  - $\boldsymbol{F}_{\text{col},p} \gg \boldsymbol{F}_{\text{other},p}$ (mostly electrostatic or Van der Waals)
  - constant m_p

$$m_p \int_{\boldsymbol{u}_p^{(0)}}^{\boldsymbol{u}_p} d\boldsymbol{u}_p = \underbrace{\int_{t_{\text{col}}}^{t_{\text{col}}+\Delta t_c} \boldsymbol{F}_{\text{col},p} dt}_{\boldsymbol{J}_p \rightarrow \text{Impulse}} \longrightarrow m_p \left(\boldsymbol{u}_p - \boldsymbol{u}_p^{(0)}\right) = \boldsymbol{J}_p$$

Trajectory (direct) collision model

- Equations:

$$m_1\left(\boldsymbol{u}_1 - \boldsymbol{u}_1^{(0)}\right) = \boldsymbol{J}_1 \equiv \boldsymbol{J}$$
$$m_2\left(\boldsymbol{u}_2 - \boldsymbol{u}_2^{(0)}\right) = \boldsymbol{J}_2 = -\boldsymbol{J}$$

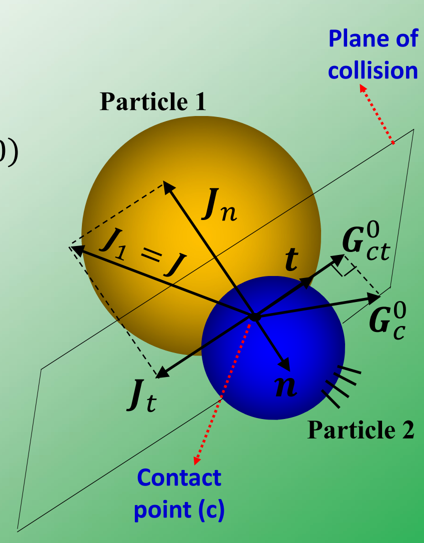
- Similarly, integrating the angular momentum equation for each particle ($p = 1$ or 2) over Δt_c, assuming
  - Negligible deformation compared to particle diameter
  - Spherical particles

$$I_1\left(\boldsymbol{\omega}_1 - \boldsymbol{\omega}_1^{(0)}\right) = \boldsymbol{r}_1 \times \boldsymbol{J}_1 = r_1 \boldsymbol{n} \times \boldsymbol{J} \qquad I_1 = \left({}^2/_5\right) m_1 r_1^2$$
$$I_2\left(\boldsymbol{\omega}_2 - \boldsymbol{\omega}_2^{(0)}\right) = \boldsymbol{r}_2 \times \boldsymbol{J}_2 = r_2 \boldsymbol{n} \times \boldsymbol{J} \qquad I_2 = \left({}^2/_5\right) m_2 r_2^2$$

Trajectory (direct) collision model

- Knowing:

$$\boldsymbol{J}_1 = \boldsymbol{J} = \boldsymbol{J}_n + \boldsymbol{J}_t = J_n \boldsymbol{n} + J_t \boldsymbol{t}$$
$$(J_n < 0, J_t < 0)$$



Trajectory (direct) collision model

- Equations (12):

$$m_1\left(\boldsymbol{u}_1 - \boldsymbol{u}_1^{(0)}\right) = J_n\boldsymbol{n} + J_t\boldsymbol{t}$$
$$m_2\left(\boldsymbol{u}_2 - \boldsymbol{u}_2^{(0)}\right) = -(J_n\boldsymbol{n} + J_t\boldsymbol{t})$$
$$\left({}^{2}\!/_{5}\right) m_1 r_1^2\left(\boldsymbol{\omega}_1 - \boldsymbol{\omega}_1^{(0)}\right) = r_1\boldsymbol{n}\times(J_n\boldsymbol{n} + J_t\boldsymbol{t})$$
$$\left({}^{2}\!/_{5}\right) m_2 r_2^2\left(\boldsymbol{\omega}_2 - \boldsymbol{\omega}_2^{(0)}\right) = r_2\boldsymbol{n}\times(J_n\boldsymbol{n} + J_t\boldsymbol{t})$$

- Unknowns (14):

$$\boldsymbol{u}_1, \boldsymbol{u}_2 \ (6)$$
$$\boldsymbol{\omega}_1, \boldsymbol{\omega}_2 \ (6)$$
$$J_n, J_t \ (2)$$

- Closure needs two additional equations
  - Two new (experimentally measured) properties

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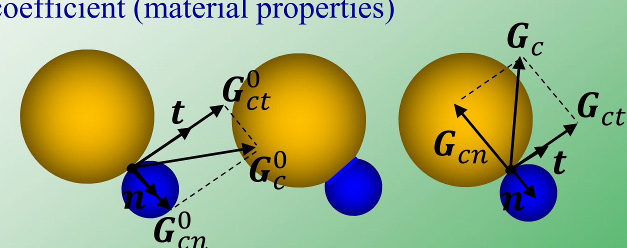
Trajectory (direct) collision model

- The first property (equation):
  - Restitution coefficient (material properties)

$$e \equiv \frac{|\boldsymbol{G}_{cn}|}{|\boldsymbol{G}_{cn}^0|}$$



  - For spherical particles with negligible deformation:

$$e = -\frac{\boldsymbol{n}.\boldsymbol{G}}{\boldsymbol{n}.\boldsymbol{G}^0} = \frac{\boldsymbol{n}.(\boldsymbol{u}_1 - \boldsymbol{u}_2)}{\boldsymbol{n}.(\boldsymbol{u}_1^0 - \boldsymbol{u}_2^0)}$$

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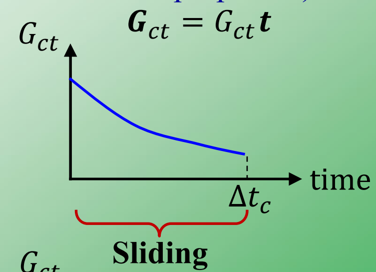
Trajectory (direct) collision model

- The second property (equation):
  - Friction coefficient (material and surface properties)

Situation 1: Continuous sliding (Coulomb's friction)

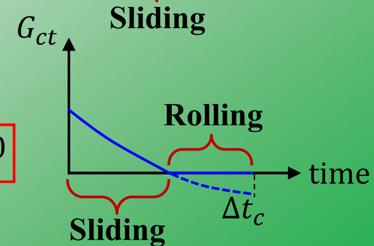
$$\boxed{J_t = f J_n}$$



Situation 2: final rolling

$\cancel{J_t = f J_n} \longrightarrow$ If $G_{ct} < 0$: $G_{ct} = 0$

or $\boxed{\boldsymbol{G} - (\boldsymbol{G}.\boldsymbol{n})\boldsymbol{n} = 0}$



Trajectory (direct) collision model

- Collision outcome: solid particles
  - The system of 14 equations and 14 unknowns can be analytically solved [2] to obtain:

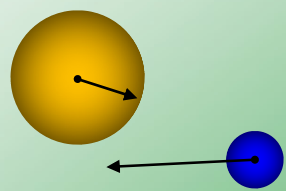
if $\dfrac{\mathbf{n}\cdot\mathbf{G}^{(0)}}{\left\lvert\mathbf{G}_{ct}^{(0)}\right\rvert} < \left(\dfrac{2}{7}\right)\dfrac{1}{f(1+e)}$:	Otherwise :
$\mathbf{v}_1 = \mathbf{v}_1^{(0)} - (\mathbf{n} + f\mathbf{t})(\mathbf{n}\cdot\mathbf{G}^{(0)})(1+e)\dfrac{m_2}{m_1+m_2}$	$\mathbf{v}_1 = \mathbf{v}_1^{(0)} - \left\{(1+e)(\mathbf{n}\cdot\mathbf{G}^{(0)})\mathbf{n} + \dfrac{2}{7}\left\lvert\mathbf{G}_{ct}^{(0)}\right\rvert\mathbf{t}\right\}\dfrac{m_2}{m_1+m_2}$
$\mathbf{v}_2 = \mathbf{v}_2^{(0)} + (\mathbf{n} + f\mathbf{t})(\mathbf{n}\cdot\mathbf{G}^{(0)})(1+e)\dfrac{m_1}{m_1+m_2}$	$\mathbf{v}_2 = \mathbf{v}_2^{(0)} + \left\{(1+e)(\mathbf{n}\cdot\mathbf{G}^{(0)})\mathbf{n} + \dfrac{2}{7}\left\lvert\mathbf{G}_{ct}^{(0)}\right\rvert\mathbf{t}\right\}\dfrac{m_1}{m_1+m_2}$
$\boldsymbol{\omega}_1 = \boldsymbol{\omega}_1^{(0)} - \left(\dfrac{5}{2r_1}\right)(\mathbf{n}\cdot\mathbf{G}^{(0)})(\mathbf{n}\times\mathbf{t})f(1+e)\dfrac{m_2}{m_1+m_2}$	$\boldsymbol{\omega}_1 = \boldsymbol{\omega}_1^{(0)} - \dfrac{5}{7r_1}\left\lvert\mathbf{G}_{ct}^{(0)}\right\rvert(\mathbf{n}\times\mathbf{t})\dfrac{m_2}{m_1+m_2}$
$\boldsymbol{\omega}_2 = \boldsymbol{\omega}_2^{(0)} - \left(\dfrac{5}{2r_2}\right)(\mathbf{n}\cdot\mathbf{G}^{(0)})(\mathbf{n}\times\mathbf{t})f(1+e)\dfrac{m_1}{m_1+m_2}$	$\boldsymbol{\omega}_2 = \boldsymbol{\omega}_2^{(0)} - \dfrac{5}{7r_2}\left\lvert\mathbf{G}_{ct}^{(0)}\right\rvert(\mathbf{n}\times\mathbf{t})\dfrac{m_1}{m_1+m_2}$

Table 1 The bouncing calculation formulation.

Trajectory (direct) collision model

- Collision outcome: solid particles
  - For every collision incidence: explicit

$$n = \mathrm{col} \rightarrow \mathrm{n} + 1$$



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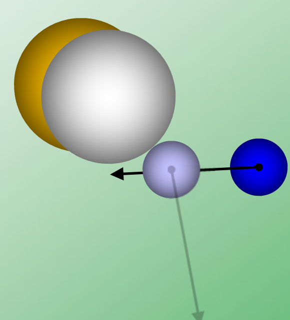
Trajectory (direct) collision model

- Collision outcome: solid particles
  - For every collision incidence: explicit

$$n = \mathrm{col} \rightarrow \mathrm{n} + 1$$



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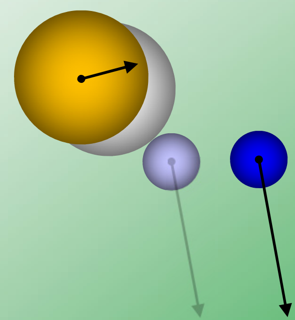
Trajectory (direct) collision model

- Collision outcome: solid particles
  - For every collision incidence: explicit

$$n = \text{col} \rightarrow \text{n} + 1$$



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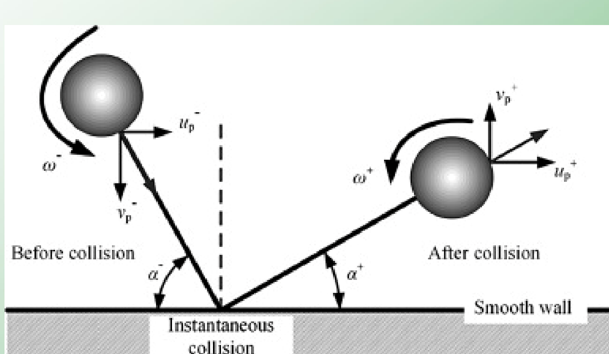
Trajectory (direct) collision model

- Particle-wall collision



$$m_2 \rightarrow \infty, r_2 \rightarrow \infty$$

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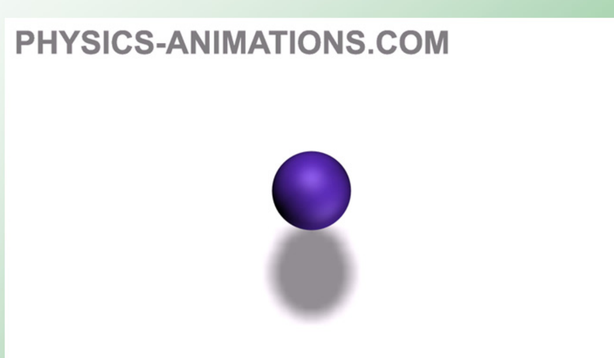
Trajectory (direct) collision model

- Sample simulations



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Trajectory (direct) collision model

- Application: elbow erosion

▲ **The role of inter-particle collision in elbow erosion**

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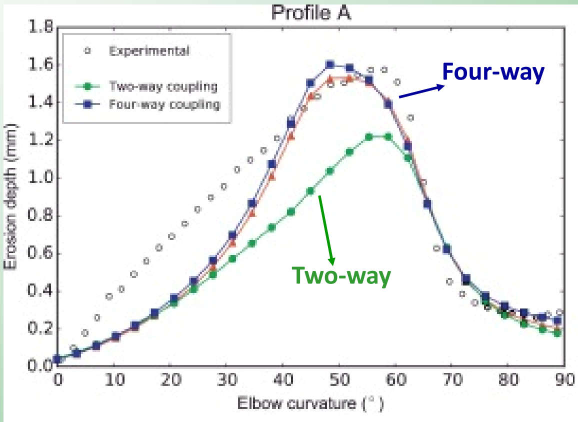
Trajectory (direct) collision model

- Application: elbow erosion



▲ The role of inter-particle collision in elbow erosion

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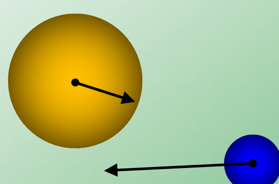
Advanced topics – collision incidence

- Collision missing: no 100% successful algorithm!



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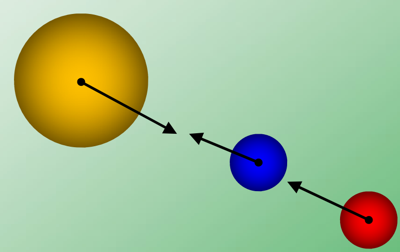
Advanced topics – collision incidence

- Collision missing: no 100% successful algorithm!
- Collision order



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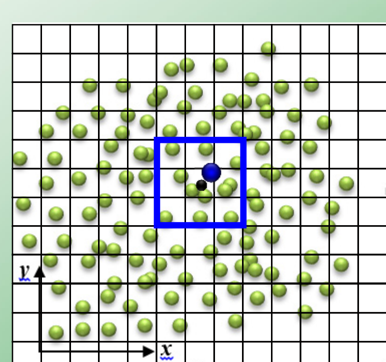
Advanced topics – collision incidence

- Collision missing: no 100% successful algorithm!
- Collision order
- Collision pair selection: region of influence



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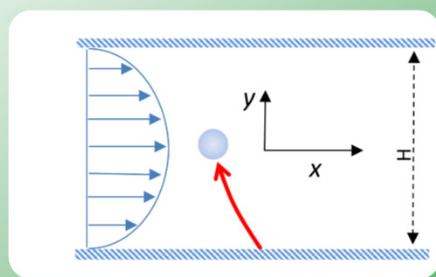
Hands-on practice

- HW#10
- Project#2-partII:
  - ✓ Adding a simple particle collision algorithm to your Lagrangian Particle Tracking (LPT) code (project#2-partI)



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