On the growth of a particle coalescing in a Poisson distribution of obstacles

Alessia Nota

University of Bonn

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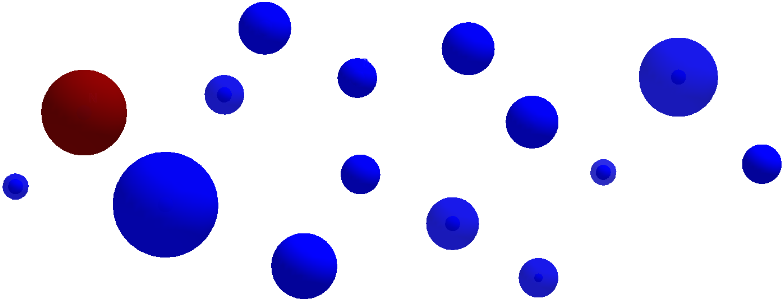
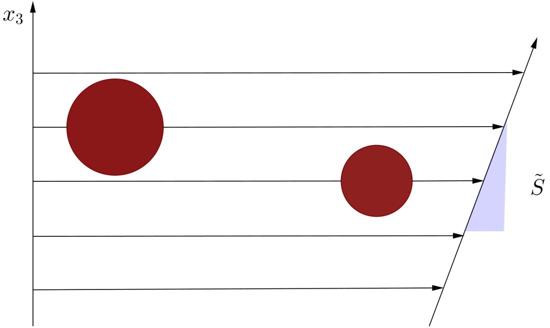
Joint work with Juan J.L. Velázquez

Young Women in Probability and Analysis, Bonn



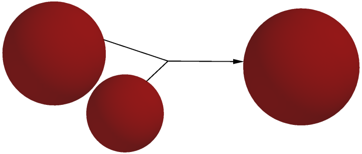
Outline

Coagulation processes in shear flows



- spherical particles in $\mathbb{R}^3$
- $u(x) = \left(\tilde{S}x_3, 0, 0\right)$ speed
  $\tilde{S} = \frac{\partial u_1}{\partial x_3}$ laminar shear coeff.

- Collisions between pairs of particles with different values of x_3
  $\Rightarrow$ instantaneous coalescence.



Smoluchowski Equation in a shear flow (1916)

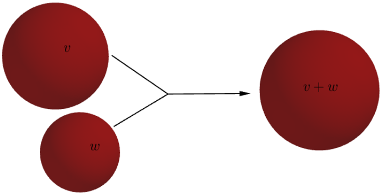
- Suitable rescaling for shear, particle density and volume fraction
  (one collision for unit of time)
- The distribution function f for the particle volume in the scaling limit satisfies

$$\partial_t f(v,t) = \frac{1}{2}\int_0^v K(v-w,w)\, f(v-w,t)\, f(w,t)\, dw - \int_0^\infty K(v,w)\, f(v,t)\, f(w,t)\, dw$$

Coagulation kernel

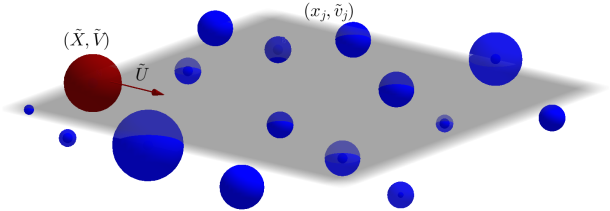
$$K(v,w) = \frac{4}{3} S (v^{\frac{1}{3}} + w^{\frac{1}{3}})^3$$

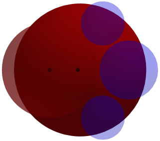
(collision frequency)



[Smoluchowski 1916]

A coalescing particle in a random background





- Random distribution of particles: $\{x_j\}_{j \in N}$ positions, $\{\tilde{v}_j\}_{j \in N}$ volumes.
- The tagged particle moves freely with speed $\tilde{U}$ along $e_1 = (1, 0, 0)$.
- Merging dynamics: the new volume is $\tilde{V} + \sum_j \tilde{v}_j$
  the new position is the center of mass.
- Average nr. of particles for unit of volume is 1.

Linear Smoluchowski Equation in a shear flow

- Suitable rescaling for the speed of the tagged particle, position and sizes. (one collision for unit of time)
- The distribution function f for the particle position and volume in the scaling limit satisfies

$$\partial_t f(Y,V,t) = U\int_0^{\frac{\pi}{2}} d\theta \int_0^{2\pi} d\varphi \Big[\int_0^V dv\, K(V-v,v,\theta) f(Y - \frac{v}{V-v} R\, n(\theta,\varphi), V-v, t) - \int_0^\infty dv\, K(V,v,\theta) f(Y,V,t)\Big] \equiv \mathcal{Q}[f](Y,V,t)$$

$$R = \left(\tfrac{3V}{4\pi}\right)^{\frac{1}{3}}, \qquad n(\theta,\varphi) = (\cos\theta, \sin\theta\cos\varphi, \sin\theta\sin\varphi)$$

$$K(V,v,\theta) = \left(\frac{3}{4\pi}\right)^{\frac{2}{3}} \sin\theta\cos\theta\, G(v)(V^{\frac{1}{3}} + v^{\frac{1}{3}})^2 \qquad \text{(coagulation kernel)}$$

The particle system (CTP model)

- $\Omega := \{\omega = \{x_k, v_k\}_{k\in I}, I \subset \mathbb{N} : \{x_k\}_{k\in I}$ loc. finite and $v_k > 0,\ x_k \in \mathbb{R}^3\}$
- $(\Omega,\ \Sigma,\ \mu_\phi)$ measure space.
  μ_ϕ s.t. $\{x_k\} \sim \mathcal{P}_1$ in $\mathbb{R}^3$ and $\{v_k\} \sim \frac{1}{\phi} G(\frac{v}{\phi})$. G prob. distr. in $[0,\infty)$.
  $\phi > 0$ volume fraction.
- $(\tilde{Y}_0, \tilde{V}_0)$ initial configuration. $\tilde{Y}(t) = \tilde{X}(t) - \tilde{U}te_1$ (moving background).
- $\tilde{T}^t(\tilde{Y}_0, \tilde{V}_0; \tilde{\omega}_0) = (\tilde{Y}(t), \tilde{V}(t); \tilde{\omega}(t))$ $t \geq 0$ (evolution flow)

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Scaling limit:

$\tilde{V} = \phi V,\ \tilde{v} = \phi v$ | mean free flight time $O(1)$

$\tilde{Y} = \phi^{\frac{1}{3}} Y,\ \tilde{U} = \phi^{-\frac{2}{3}} U$ $\rightsquigarrow$ mean free path $O(\phi^{-\frac{2}{3}})$

$\Rightarrow \quad T^t_\phi(Y_0, V_0; \omega_0) = (Y(t), V(t); \omega(t)) \quad$ (CTP model)

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$\mathcal{F}(Y, V, t^*) \in \Sigma$ free flow in $[0, t^*]$, $\quad \mathcal{C}(Y, V, t^*) \in \Sigma$ collisions at $t^* \geq 0$

$$\mathcal{A}_{\omega \in \mathcal{C}}(Y, V; \omega) = \left(\frac{VY + \sum_{k \in J} x_k v_k}{V + \sum_{k \in J} v_k}, V + \sum_{k \in J} v_k; \omega \setminus J \right)$$ merging operator

Definition of the flow

1. If $\omega(\bar{t}) \in \mathcal{F}(Y(\bar{t}), V(\bar{t}), t^*)$ for some $t^* > \bar{t}$

   $\Rightarrow \quad (Y(t), V(t); \omega(t)) = (Y(\bar{t}), V(\bar{t}); \omega(\bar{t})) \quad \forall t \in [\bar{t}, t^*]$

2. Set $(Y^0, V^0; \omega^0) = (Y(t^-), V(t^-); \omega(t^-))$. $(Y^1, V^1; \omega^1) = \mathcal{A}(Y^0, V^0; \omega^0)$.

   $\Rightarrow$
   1) if $\omega^1 \in \mathcal{F}(Y_1, V_1, t) \Rightarrow$ free flow (step 1)
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2.2) for n large $\Rightarrow$ the dynamics stops at $t < \infty$ with infinite seq. of coalescences !

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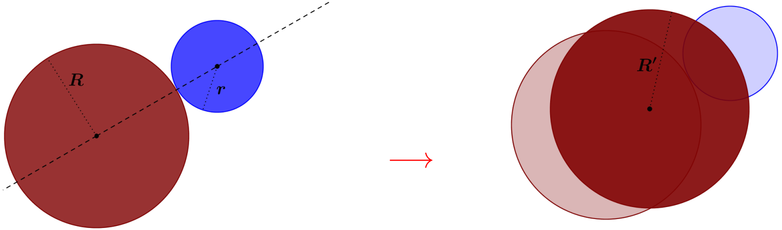
Kinematic of binary collisions



$V = \frac{4}{3}\pi R^3,\ v = \frac{4}{3}\pi r^3$ $\qquad$ $(V, v) \to V + v,\ \ R' = (r^3 + R^3)^{\frac{1}{3}}$

Coalescing dynamics $\rightsquigarrow$ position of the center of mass of the new particle?

$x = X + (\cos\theta\, \vec{e}_1 + \sin\theta\, \vec{\nu})\,(R + r)$ $\qquad$ (position of the centre of the obstacle)

$\vec{\nu} = \vec{\nu}(\varphi) = (0, \cos\varphi, \sin\varphi),\ \varphi \in [0, 2\pi],\quad \theta \in [0, \frac{\pi}{2}].$

$$X' = X + \frac{v}{V + v}(\cos\theta \vec{e}_1 + \sin\theta\, \vec{\nu})(R + r), \quad V' = V + v$$

Comments....

Ass : $\int_0^\infty G(v)\, v^\gamma dv < \infty \;\; \gamma > 2$ (the number of big obstacles is not too large!)

- $\int_0^\infty G(v)\, v^{\frac{5}{3}} dv < \infty \Rightarrow \exists\, \phi_* > 0$ (critical vol. frac.) s.t. for $0 < \phi < \phi_*$

  all the clusters of particles are finite with prob. one.

  (*Continuum Percolation Theory*)

  [Hall '85; Grimmett '99; Meester, Roy '96]

Main difficulties

- coalescing particles could trigger sequences of coagulation events
  $\rightsquigarrow$ formation of an infinite cluster
- the free flights between coagulation events become shorter (increasing volume)
  $\rightsquigarrow$ runaway growth of the tagged particle in finite time.

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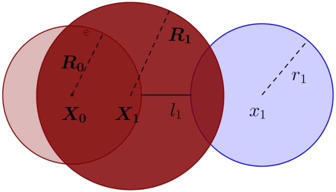
Blow-up?

Finite nr. of steps for all the coag. events $\Rightarrow$ global well-posedness ?

No! Blow-up in finite time might happen if $\{\tau_j\}$ is s.t. $\sum_{j\geq 1} \tau_j < \infty$

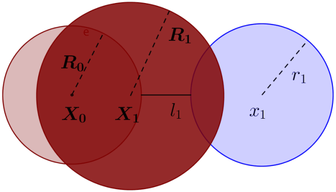
Example



- $\{l_j\}_j$ s.t. $l_j > 0$ and $\sum_{j\geq 1} l_j < \infty$
- $X_0 = 0,\ V_0 = 1,\ \|U\| = 1;\quad v_k = 1\ \forall k,\ \ x_k \vec{e}$ s.t.

$$x_{k+1} = x_k + \left(\frac{3}{4\pi}\right)^{\frac{1}{3}}\left((k+1)^{\frac{1}{3}} - \frac{(1+k^{\frac{1}{3}})k}{k+1} + 1\right) + l_{k+1} \quad k \geq 0, \qquad x_0 = 0.$$

Blow up example



- At the collision times $\tau_j = \sum_{k=1}^{j} l_k$

$$V_j = j+1, \quad R_j = \left(\frac{3}{4\pi}(j+1)\right)^{\frac{1}{3}}$$

$$X_j = x_j - \frac{V_{j-1}}{V_j}\left(\left(\frac{3}{4\pi}(j+1)\right)^{\frac{1}{3}} + R_j\right)$$

$$\Downarrow$$

At $T = \sum_{j=1}^{\infty} l_j < \infty$ the volume of the tagged particle becomes infinite !

Global well-posedness

If...

1. the coalescence events have a finite number of steps with probability one
2. the total length of the free flights of the tagged particle is infinite with probability one ($\sum_j l_j = \infty$)

$\Rightarrow$ the motion of the tagged particle is defined globally in time.

Theorem [N., Velázquez '16]

$G \in \mathcal{M}_+([0,\infty))$ s.t. $\mathrm{supp}\,(G(\cdot)) \in [0, v_*]$.

There exists $\phi_* = \phi_*(v_*) > 0$ s.t. $\forall\, \phi \leq \phi_*$ and $\forall\, (Y_0, V_0) \in \mathbb{R}^3 \times [0,\infty)$

$\Rightarrow \exists\, \tilde{\Omega} \subset \Omega,\ \tilde{\Omega} \in \Sigma$ s.t. $\mathbb{P}(\tilde{\Omega}) = 1$

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Rigorous derivation of the kinetic equation

Setting: $\mathcal{P} := \mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^+)$ probability measures on $\mathbb{R}^3 \times \mathbb{R}^+$

$\mathcal{M}_+ := \mathcal{M}_+(\mathbb{R}^3 \times \mathbb{R}^+)$ Radon measures on $\mathbb{R}^3 \times \mathbb{R}^+$.

Solution of the microscopic coalescence process

$f_0 \in \mathcal{P}$. For any Borel set A of $\mathbb{R}^3 \times \mathbb{R}^+$ we define $f_\phi \in L^\infty([0,T); \mathcal{M}_+)$ as

$$\int_A f_\phi(Y,V,t)dY\,dV = \int_{\mathbb{R}^3\times\mathbb{R}^+} \mu_\phi(\{\omega \,:\, \Pi[T^t_\phi(Y_0,V_0;\omega)] \in A\}) f_0(Y_0,V_0)dY_0\,dV_0$$

Solutions of the equation in the sense of measures

$f \in C([0,T]; \mathcal{M}_+)$ is a weak solution if $f_0 \in \mathcal{P}$ and $\forall\, \Psi \in C^1_c([0,T)\times\mathbb{R}^3\times[0,\infty))$

$$-\int_0^T\int_{\mathbb{R}^3\times\mathbb{R}^+} f(Y,V,t)\{\partial_t\Psi(Y,V,t)+\mathcal{C}[\Psi](Y,V,t)\}dYdVdt = \int_{\mathbb{R}^3\times\mathbb{R}^+} f_0(Y,V)\Psi_0(Y,V)dYdV$$

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$f_0 \in \mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^+)$, $f_\phi \in L^\infty([0,T);\mathcal{M}_+(\mathbb{R}^3 \times \mathbb{R}^+))$ and $T > 0$

$\Rightarrow$ $\forall\, A \in \mathbb{R}^3 \times \mathbb{R}^+$ $\quad \int_A f_\phi(t) \underset{\phi \to 0}{\longrightarrow} \int_A f(t)$ $\quad$ uniformly in $[0,T]$

where f is the unique weak solution of the lin. Smoluchowski eq.

Pb: the particle dynamics is not time reversible!

Trick: instead of the forward Kolmogorov eq. for the probability density $f(Y,V,t)$ consider the backward Kolmogorov eq. for a test function $\Psi(Y,V,t)$

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$\Rightarrow \qquad \forall\, A \in \mathbb{R}^3 \times \mathbb{R}^+ \qquad \int_A f_\phi(t) \underset{\phi \to 0}{\longrightarrow} \int_A f(t) \qquad$ uniformly in $[0, T]$

where f is the unique weak solution of the lin. Smoluchowski eq.

Pb: the particle dynamics is not time reversible!

Trick: instead of the forward Kolmogorov eq. for the probability density $f(Y, V, t)$ consider the backward Kolmogorov eq. for a test function $\Psi(Y, V, t)$

$$\partial_t \Psi(Y, V, t) = (\mathcal{C}[\Psi])(Y, V, t)$$

$$\int_{\mathbb{R}^3 \times \mathbb{R}^+} f(Y, V, t)\psi(Y, V, 0)\, dY dV = \int_{\mathbb{R}^3 \times \mathbb{R}^+} f(Y, V, 0)\psi(Y, V, t)\, dY dV$$

The adjoint problem

- The backward Kolmogorov equation

$$
\begin{aligned}
\partial_t \Psi(Y,V,t) = {} & U \int_0^{\infty} dv \int_0^{\frac{\pi}{2}} d\theta \int_0^{2\pi} d\varphi \, G(v)(R+r)^2 \sin\theta \cos\theta \\
& \left[\Psi\left(Y + \frac{v}{V+v} n(\theta,\varphi)(R+r), V+v, t\right) - \Psi(Y,V,t) \right] = (\mathcal{C}[\Psi]) \\
= {} & U\,(\mathrm{K}[\Psi])\,(Y,V,t) - U\lambda(V)\Psi(Y,V,t)
\end{aligned}
$$

- Duhamel's representation formula for the unique solution

$$
\begin{aligned}
\Psi(Y,V,t) = {} & \Psi_0(Y,V)\, e^{-U\lambda(V)t} + \sum_{n>0} U^n \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 \\
& \left[e^{-U\lambda(\cdot)(t-t_n)} \mathrm{K}\, e^{-U\lambda(\cdot)(t_n-t_{n-1})} \mathrm{K} \dots \mathrm{K}\, e^{-U\lambda(\cdot)(t_1)} \Psi_0(\cdot) \right] (Y,V)
\end{aligned}
$$

Main Steps

1. The probability of the set of good configurations tends to one when $\phi \to 0$

   - $\Omega = \underbrace{\Omega^1}_{\textit{good conf.}} \cup \underbrace{\Omega^2}_{\textit{bad conf.}}$, Ω^1 set of well separated configurations

   For any $\delta > 0$ there exists $\varepsilon_* = \varepsilon_*(\delta, T) > 0$ s.t. if $\varepsilon_0 \in (0, \varepsilon_*)$ and $\phi < \varepsilon_0^\beta$

   $$\Rightarrow \qquad \mathbb{P}(\Omega^1) \geq 1 - \delta \qquad \forall\ V_0 \in [0, M]$$

2. Convergence for the adjoint problem

   - $\Psi_\phi(Y, V, t) := \mathbb{E}_{\mu_\phi}[\Psi_0(\Pi\left[T^t(Y, V; \omega)\right])]$, $\quad \Psi_0$ smooth.

   $$\lim_{\phi \to 0} \Psi_\phi(Y, V, t) = \Psi(Y, V, t) \quad \text{in} \quad C([0, T]; C_b(\mathbb{R}^3 \times \mathbb{R}^+))$$

   [Constructive approach]

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   [Constructive approach]

Long time behaviour for the distribution of volumes

- Assume $G(v)$ decreasing fast enough $\left[\int_0^\infty G(v) v^{\frac{5}{3}+\theta} dv < \infty,\ \theta > 0\right]$
- $F(V,t) := \int_{\mathbb{R}^3} dY f(Y,V,t)$ (average of f with respect to Y) satisfies

$$\partial_t F(V,t) = \lambda\Big(\int_0^V dv\, G(v)((V-v)^{\frac{1}{3}} + v^{\frac{1}{3}})^2 F(V-v,t) - \int_0^\infty dv\, G(v)(V^{\frac{1}{3}} + v^{\frac{1}{3}})^2 F(V,t)\Big)$$

$$\Downarrow$$

$F(Wt^3,t)t^3 \overset{*}{\rightharpoonup} \delta(W-a)$ as $t \to \infty$ in $\mathcal{M}_+(\mathbb{R}^+)$, $\quad a = \frac{\lambda^3}{27}\left(\int_0^\infty v\, G(v)\, dv\right)^3$

- The volume of the tagged particle increases like $a\, t^3$ as $t \to \infty$

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Perspectives & future targets

- Analysis of the long time asymptotics for the solution of

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  according to the choice of $G(v)$ (different regimes for different power laws)

- Rigorous derivation of the Smoluchowski equation

  (particles in a laminar shear flow)

$$\partial_t f(v,t) = \frac{1}{2}\int_0^v K(v-w,w) f(v-w,t) f(w,t)\,dw - \int_0^\infty K(v,w) f(v,t) f(w,t)\,dw$$

$$K(v,w) = \frac{4}{3} S(v^{\frac{1}{3}} + w^{\frac{1}{3}})^3$$

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Thanks for your attention !

The evolution flow

Let be $t^* \geq 0$. We define the sets

- $\mathcal{F}(Y, V, t^*) \in \Sigma$ as

$$\mathcal{F}(Y, V, t^*) := \{\omega \in \Omega \,:\, \inf_{k:\{(x_k, r_k)\}=\omega} |Y - (x_k - Ut^* e_1)| > \sigma(V^{\frac{1}{3}} + v_k^{\frac{1}{3}})\}.$$

- $\mathcal{C}(Y, V, t^*) \in \Sigma$ as

$$\mathcal{C}(Y, V, t^*) = \{\omega \in \Omega \,:\, \inf_{k:\{(x_k, r_k)\}=\omega} |Y - (x_k - Ut^* e_1)| \leq \sigma(V^{\frac{1}{3}} + v_k^{\frac{1}{3}})\}.$$

Here $\sigma = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}}$.

Convergence for the adjoint problem (step 2)

$$\Psi_\phi(Y,V,t) = \underbrace{\mathbb{E}_{\mu_\phi}[\chi_{\text{good}}(\omega)\Psi_0(\Pi\big[T^t(Y,V;\omega)\big])]} \quad + \underbrace{\mathbb{E}_{\mu_\phi}[\chi_{\text{bad}}(\omega)\Psi_0(\Pi\big[T^t(Y,V;\omega)\big])]}_{\leq \|\Psi_0\|_\infty\,\delta}$$

$$\downarrow$$

$$e^{-|\mathcal{B}|}\sum_{N\geq 0}\frac{1}{N!}\int_{\mathcal{B}^N} d\mathbf{y}_N \int_{[0,\infty)^N} d\mathbf{w}_N G(\mathbf{w}_N)\chi_{\text{good}}(\omega)\chi(\{\omega\in\Omega : \#\omega_{|_{\mathcal{B}}} = n\})\Psi_0(\Pi\big[T^t(Y,V;\omega)\big])$$

Strategy: constructive approach [Gallavotti '79]

Key tools: suitable change of variables $\rightsquigarrow$ construct a trajectory in $[t_i, t_{i+1}]$, $i\in[0,n]$

$$0\leq t_1 < t_2 < \cdots < t_n \leq t$$
$$x_1,\ldots,x_n \longrightarrow t_1,\beta_1,\ldots,t_n,\beta_n$$

$\beta_i = \beta_i(\theta_i,\varphi_i)$ "collision parameters", t_i entrance time

Rk: restriction to $\Omega_1 \Rightarrow$ no need to define the flow with multiple collisions

Sequence of coagulation events and free flights

For any $\omega \in \Omega$ and (X_0, V_0) initial condition define a sequence

$$(\underline{x}^{1,1}, \underline{v}^{1,1}; \underline{x}^{1,2}, \underline{v}^{1,2}; \ldots; \underline{x}^{1,m_1}, \underline{v}^{1,m_1}; l_1, \beta_1, w_1; \underline{x}^{2,1}, \underline{v}^{2,1}; \underline{x}^{2,2}, \underline{v}^{2,2}; \ldots; \underline{x}^{2,m_2}, \underline{v}^{2,m_2}; l_2, \beta_2, w_2; \ldots)$$

$$\underline{x}^{j,l} = \{\underbrace{x_1^{j,l}}_{\in\mathbb{R}}, \ldots, x_{n_{j,l}}^{j,l}\}; \ \underline{v}^{j,l} = \{\underbrace{v_1^{j,l}}_{\in\mathbb{R}^+}, \ldots, v_{n_{j,l}}^{j,l}\}; \ l_k > 0; \ \beta_k \in S^2, \ w_k \geq 0$$

- $(\underline{x}^{j,l}, \underline{v}^{j,l})$: set of particles coalescing at any single step.
  $[\underline{x}^{j,l}, \underline{v}^{j,l}]$: coagulation type step. $[l_k, \beta_k, w_k]$ flight type step.
  l_k: length of a free flight. $\beta_k = \cos\theta e_1 + \sin\theta\,\nu$.
  w_k: vol. of the obst. colliding with the tagged particle after the free flight.

Coalescence events $=$ a sequence of coalescence steps between free flights

- Collisions at the end of a free flight are only binary collisions with probability one.
- The probability of multiple collisions during a coalescence step is strictly positive.