UNIVERSITY of DELAWARE

Collision efficiency of cloud droplets: Results from point-droplet to droplet-resolving simulations

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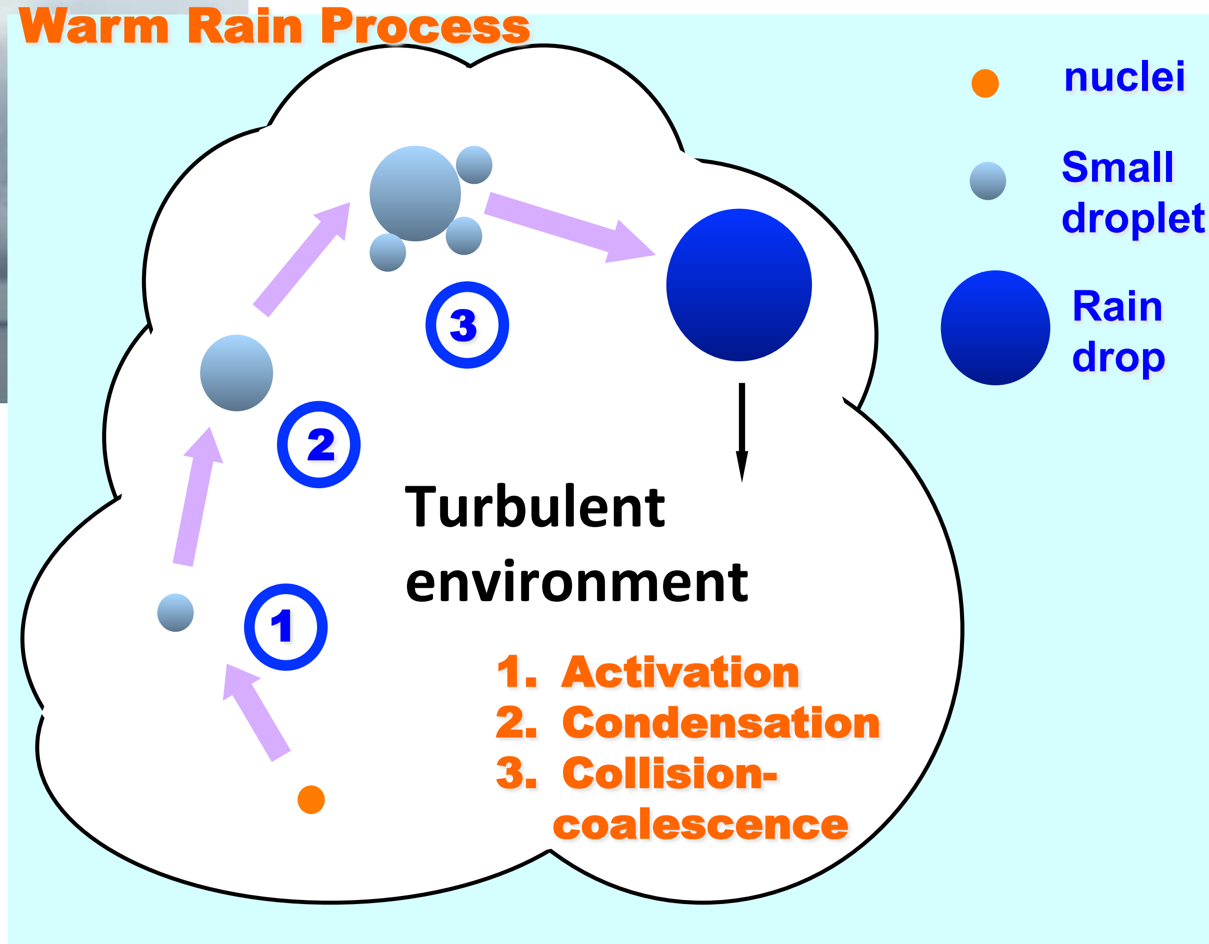
Indian Institute of Tropical Meteorology, Ministry of Earth Science, Pune, India

Outline

- Background and Motivation
- Overview of point-droplet based hybrid direct numerical simulations
  - A status report
  - Open research
- Droplet-resolving direct numerical simulations
  - Why do we need it?
  - Is it possible?
  - Results for the case of gravitational coalescence
- Summary

Collision-coalescence: effects of small-scale turbulence on the 3rd microphysical step to warm rain initiation

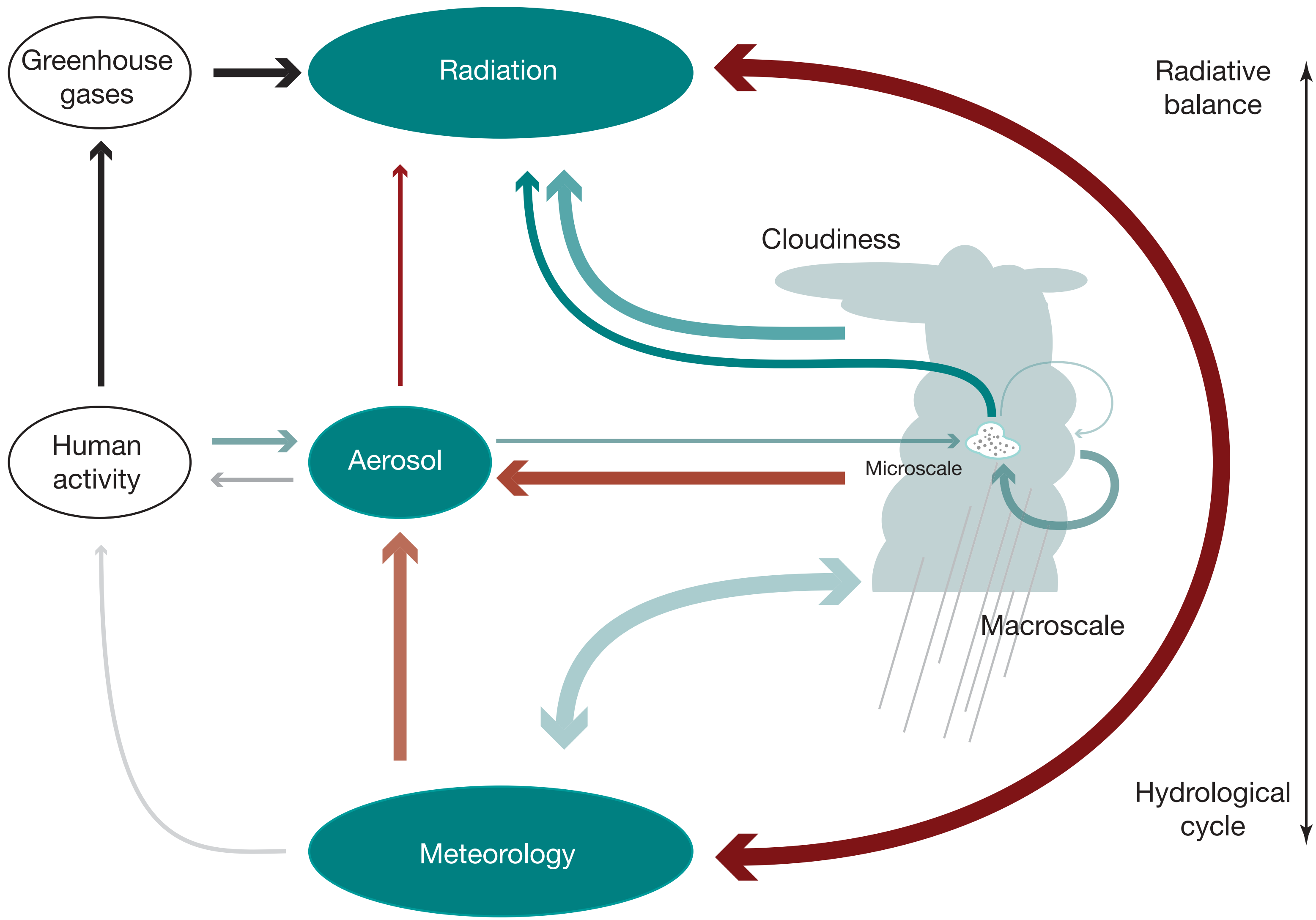
Growth of cloud droplets



How does air turbulence affect the collision rates and collision efficiency of cloud droplets?

What is the impact on warm rain initiation?

Aerosol-cloud-weather/climate interactions

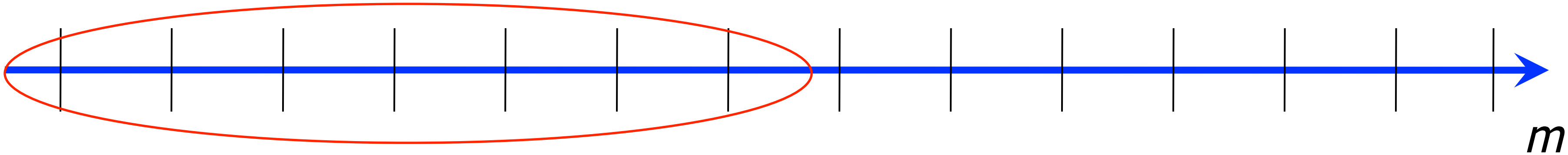


Stevens and Feingold, 2009, Nature, 461, doi:10.1038.

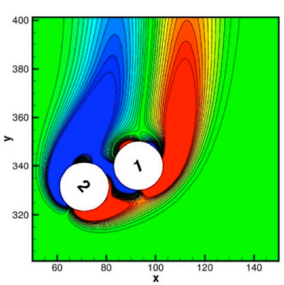
Cloud physics: The multiscale problem down to droplet size!

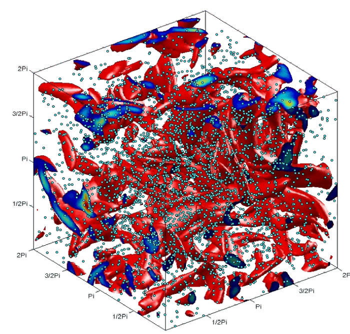
Cloud microphysics | Cloud dynamics

Droplet-resolving | **Turbulence-resolving** | **Cloud-resolving** | **Mesoscale** | **Global**



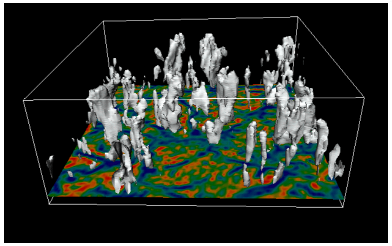
Droplet-resolving DNS | Hybrid DNS | LES | NWP | GCM

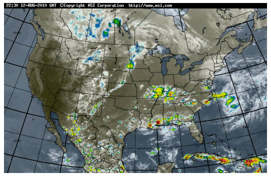




~ 1 km

cloud-scale flow



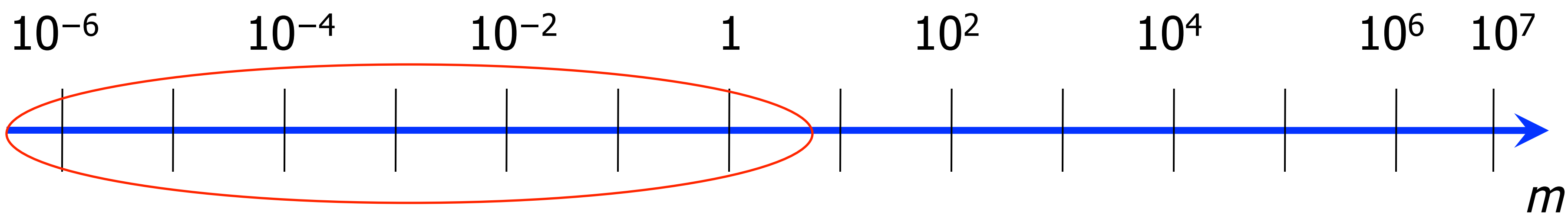


C.-H. Moeng, NCAR

Cloud physics: Also a wide range of time scales

Cloud microphysics | Cloud dynamics

Droplet-resolving | **Turbulence-resolving** | **Cloud-resolving** | **Mesoscale** | **Global**



Droplet-resolving DNS | Point-droplet hybrid DNS | LES | NWP | GCM

$$\tau_p = \frac{2\rho_p a^2}{9\mu}$$

$\approx 0.1\ ms \rightarrow 10\ ms$

$$\frac{10(a_1 + a_2)}{\Delta W}$$

$\approx 1\ ms \sim 100\ ms$

$\tau_K \approx$ $10ms \sim 100ms$

$T_e \sim 100\ s$

hours

days

←Overlap of droplet inertial response time and droplet-pair interaction time

General comments on the warm rain process

Fluid dynamics: a process driven by at least three levels of nonlinearity

Nonlinear advection, momentum-buoyancy coupling, local heating due to condensation

- Large flow Reynolds number
- Vertical Buoyancy velocity scale ~ horizontal wind fluctuations
- Latent heat release ~ kinetic energy of turbulent air flow

Multiscale processes: Coupling of microphysics and turbulent flows

- Dispersed multiphase turbulent flow with phase change

Clouds are the major source of uncertainty in weather prediction

We understand warm rain process well *qualitatively*

The devil is in the *quantitative* details and complex couplings among scales

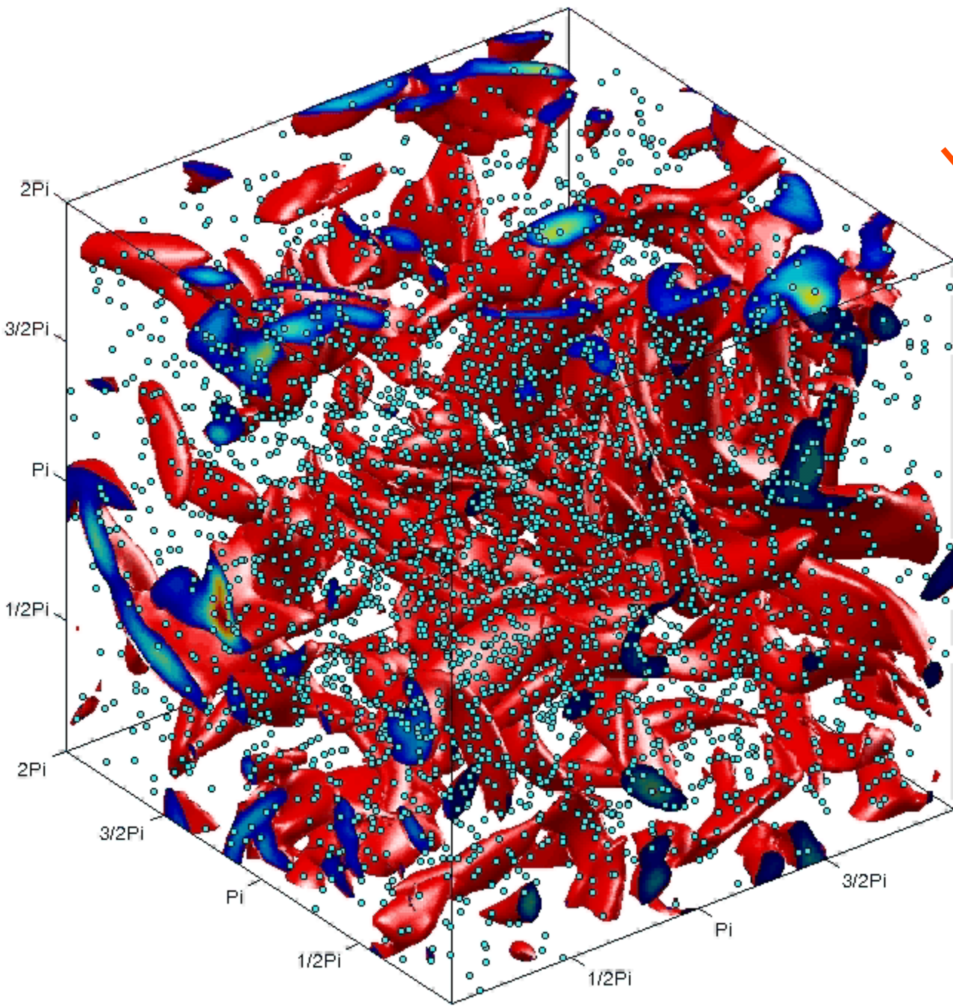
The spectral width of cloud droplets?

The time scale for warm rain initiation?

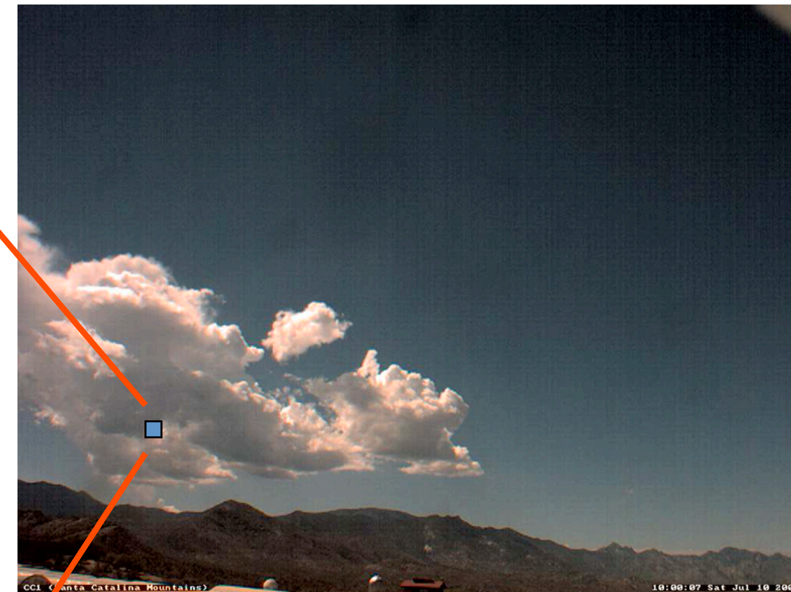
…..

Effect of air turbulence on collision-coalescence?

Hybrid Direct Numerical Simulation



Real clouds

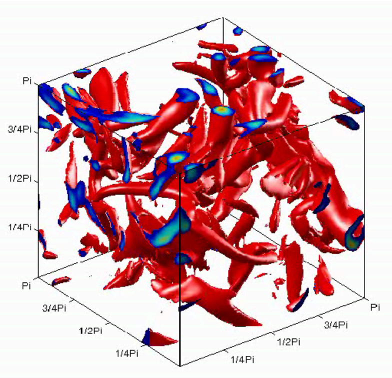


Grabowski and Wang, Growth of cloud droplets in a turbulent environment. *Annu. Rev. Fluid Mech.*, 45 (2013) 293-324.

Direct simulation of small-scale air turbulence: A bottom-up approach

Flow field

$$\frac{\partial \vec{U}}{\partial t} = \vec{U} \times \vec{\omega} - \nabla\left(\frac{P}{\rho} + \frac{1}{2}U^2\right) + \nu \nabla^2 \vec{U} + \vec{f}(\vec{x}, t)$$



solved with $\nabla \cdot \vec{U} = 0$ in a periodic box

isotropic and homogeneous: $\langle \vec{U}(\vec{x}, t) \rangle = 0$

Kolmogorov scales:

$$\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}; \quad \tau_k = \left(\frac{\nu}{\varepsilon}\right)^{1/2}; \quad v_k = (\nu\varepsilon)^{1/4}$$

Primary effect

Effect of large scales:

$$u' = \sqrt{\frac{\langle \vec{U} \cdot \vec{U} \rangle}{3}} \quad \text{or} \quad R_\lambda = \sqrt{15}\left(\frac{u'}{v_k}\right)^2$$

Secondary effect

Small-scale flow of adiabatic cumulus cloud core is assumed to be nearly homogeneous and isotropic. (Vaillancourt and Yau 2000)

One-way coupling: Loading $= O(10^{-3})$ by mass or $O(10^{-6})$ by volume.

Equation of motion for droplets

$$\frac{d\vec{V}^{(\alpha)}(t)}{dt} = -\frac{\vec{V}^{(\alpha)}(t) - \left[\vec{U}\left(\vec{Y}^{(\alpha)}(t),t\right) + \vec{u}(\vec{Y}^{(\alpha)},t)\right]}{\tau_p^{(\alpha)}} - \vec{g}$$

$$\frac{d\vec{Y}^{(\alpha)}(t)}{dt} = \vec{V}^{(\alpha)}(t)$$

Where $\tau_p^{(\alpha)} = 2\rho_p\left(a^{(\alpha)}\right)^2/(9\mu)$, $W^{(\alpha)} = \tau_p^{(\alpha)} g$

If hydrodynamic interaction is considered: $\vec{u}(\vec{Y}^{(\alpha)},t) \neq 0$

Self-consistent: no ambiguity in defining undisturbed fluid velocity

Typically tracking $10^5 \sim 10^7$ droplets with hydrodynamic interactions.

A lot of quantitative information can be extracted!

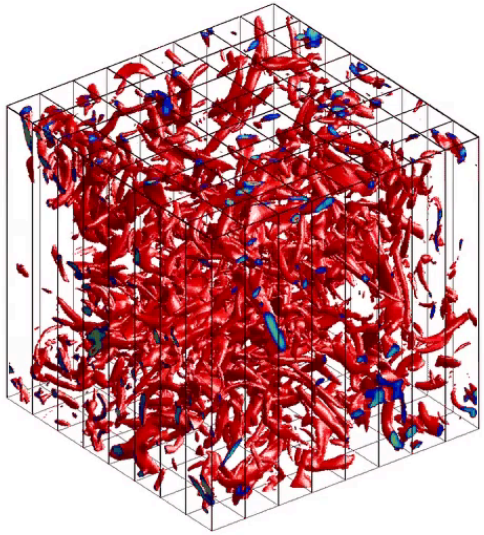
The hybrid DNS approach: disturbance flows due to droplets

$$\vec{U}(\vec{x},t)+\sum_{m=1}^{N_p}\vec{u}_s\left(\vec{Y}-\vec{Y}^{(m)};a^{(m)},\vec{V}^{(m)}-\vec{U}\left(\vec{Y}^{(m)},t\right)-\vec{u}^{(m)}\right)$$

Three-way interactions?

Background turbulent flow

Disturbance flows due to droplets



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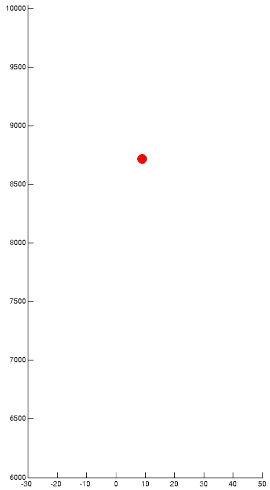
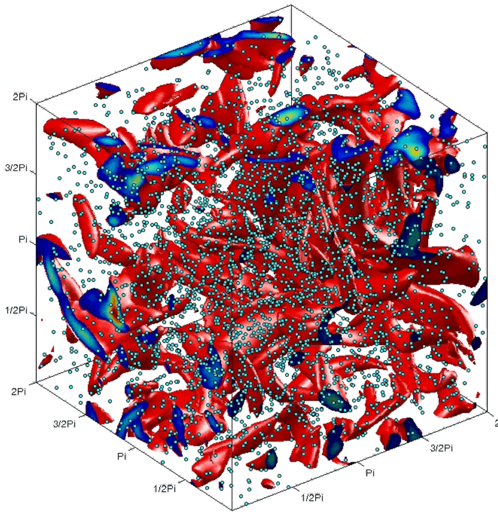




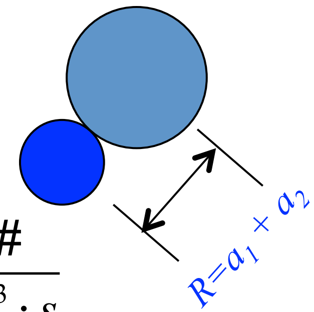
Features: Background turbulent flow can affect the disturbance flows;
No-slip condition on the surface of each droplet is satisfied on average;
Both near-field and far-field interactions are considered;
Approximate method but efficient.

Wang, Ayala, and Grabowski, J. Atmos. Sci. 62(4): 1255-1266 (2005).
Ayala, Wang, and Grabowski, J. Comp. Phys, 225, 51-73 (2007).
Onishi, Takahashi, Vassilicos, J. Comp. Phys, 242, 809-827 (2013).

Dynamic collision kernel

Volume concentrations are low, binary collision events dominate

$$\Gamma_{12}^{D} = \frac{\langle \dot{N}_{12} \rangle}{\langle n_1 \rangle \cdot \langle n_2 \rangle}$$



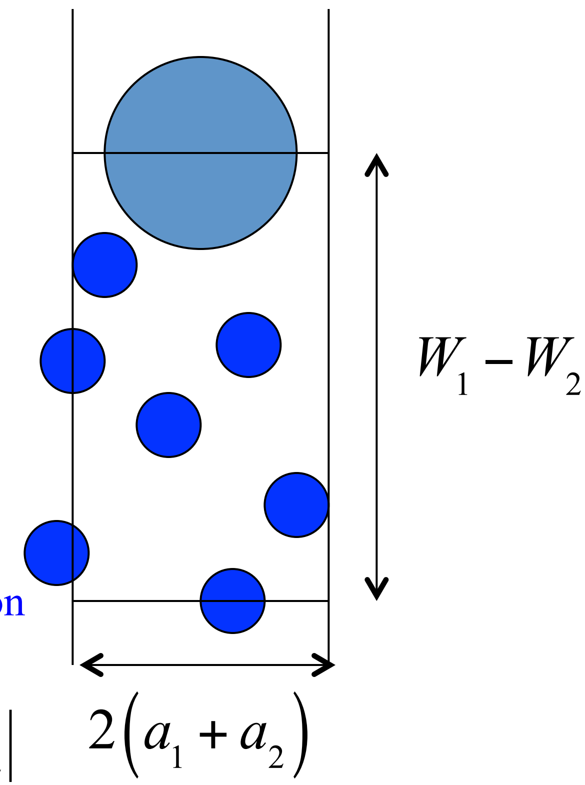
Much more complex:
Turbulence
Droplet inertia
Hydrodynamic interaction

$$\langle \dot{N}_{12} \rangle = \frac{\#\ \text{of collision events}}{(\text{per unit volume})\cdot(\text{per unit time})} = \frac{\#}{m^3 \cdot s}$$

$$\langle n_1 \rangle = \frac{\#\ \text{of particles of radius}\ a_1}{(\text{per unit volume})} = \frac{\#}{m^3}$$

$$\langle n_2 \rangle = \frac{\#\ \text{of particles of radius}\ a_2}{(\text{per unit volume})} = \frac{\#}{m^3}$$

$$\Rightarrow \quad \Gamma_{12}^{D} = \frac{m^3}{s} = \frac{\text{relative swept volume}}{\text{time}}$$



Kinematic description →
No hydrodynamic interaction
No turbulence

$$\Gamma_{12}^{K} = \pi \left(a_1 + a_2\right)^2 \left|\mathrm{W}_1 - \mathrm{W}_2\right|$$

Geometric collision kernel: Finite-inertia droplets in a turbulent flow

$$\Gamma_{12} = \frac{\dot{N}}{\langle n_1 \rangle \langle n_2 \rangle} = 2\pi R^2 \langle | w_r(r=R) | \rangle g_{12}(r=R)$$

Geometric Radial relative velocity

Geometric radial distribution function

$$\langle | w_r | \rangle = \frac{1}{N_{pair}} \sum_{all\ pairs} \left| \vec{r} \cdot \frac{(\vec{V}_1 - \vec{V}_2)}{r} \right|$$

$$g_{12}(R) = \lim_{\delta << r} \frac{N_{pair}(r-\delta \le d \le r+\delta) / 4\pi\left[(r+\delta)^3 - (r-\delta)^3\right]}{N_1 N_2 / V_B}$$

- Based on the spherical formulation
- Confirmed by DNS for all different situations
- Straightforward to calculate in DNS, but could be very difficult to measure!!!

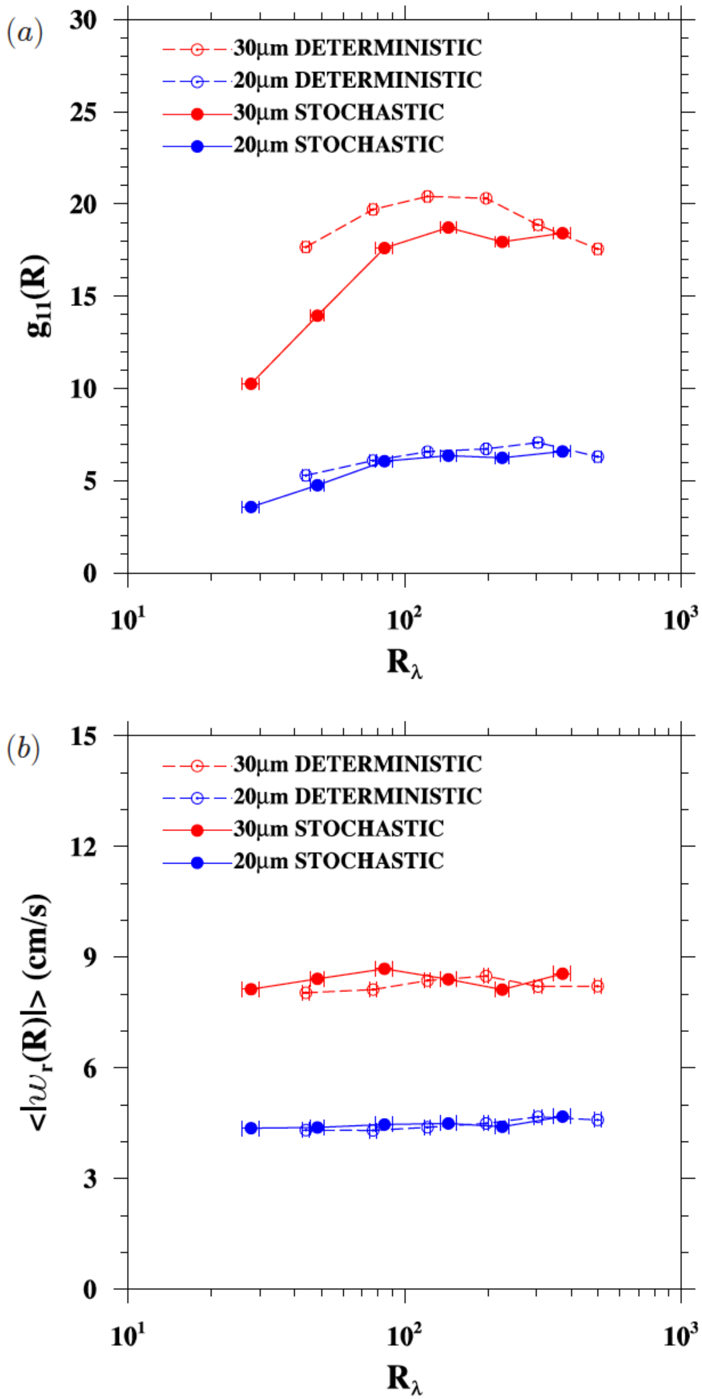
Sundaram & Collins, J. Fluid Mech. 335: 75-109 (1997).
Wang, *et al.* J. Atmos. Sci. 62: 2433-2450 (2005).

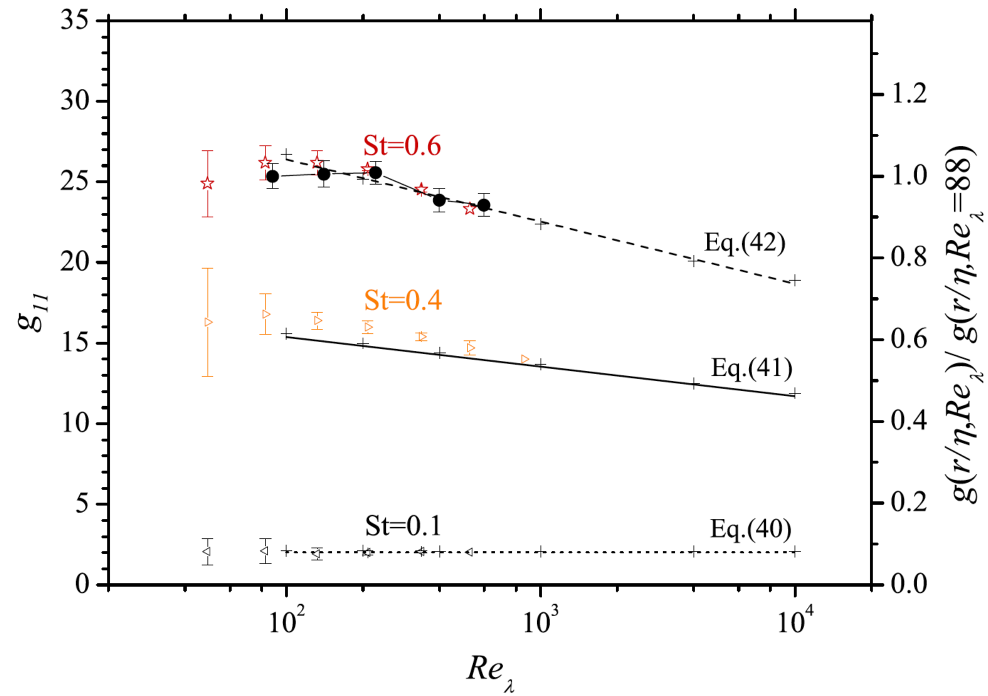
Representative results on the geometric collision rate of cloud droplets

	(a_1, a_2) (μm)	ε $(cm^2 s^{-3})$	R_λ	Resolution
Franklin et al. (2005, 2007)	2.5 ~ 30	95 ~ 1535	up to 55	240^3
Wang et al. (2005) Ayala et al. (2008a,b)	10 ~ 60	10 ~ 400	up to 72	128^3
Rosa et al. (2013)	10 ~ 60	400	up to 500	1024^3
Chen et al. (2016)	5 ~ 25	50 ~ 1500	up to 589	1024^3
Onishi & Seifert (2016)	20 ~ 50	100 ~ 1000	up to 1140	6000^3

Analytical parameterizations are made available.

Reynolds number dependence



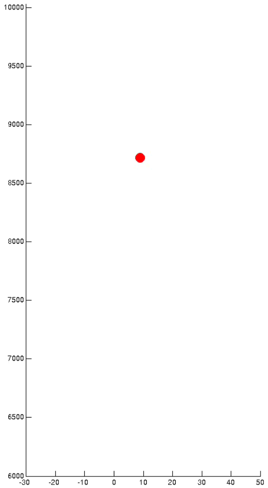


Onishi and Seifert (2016) Atmos. Chem. Phys.

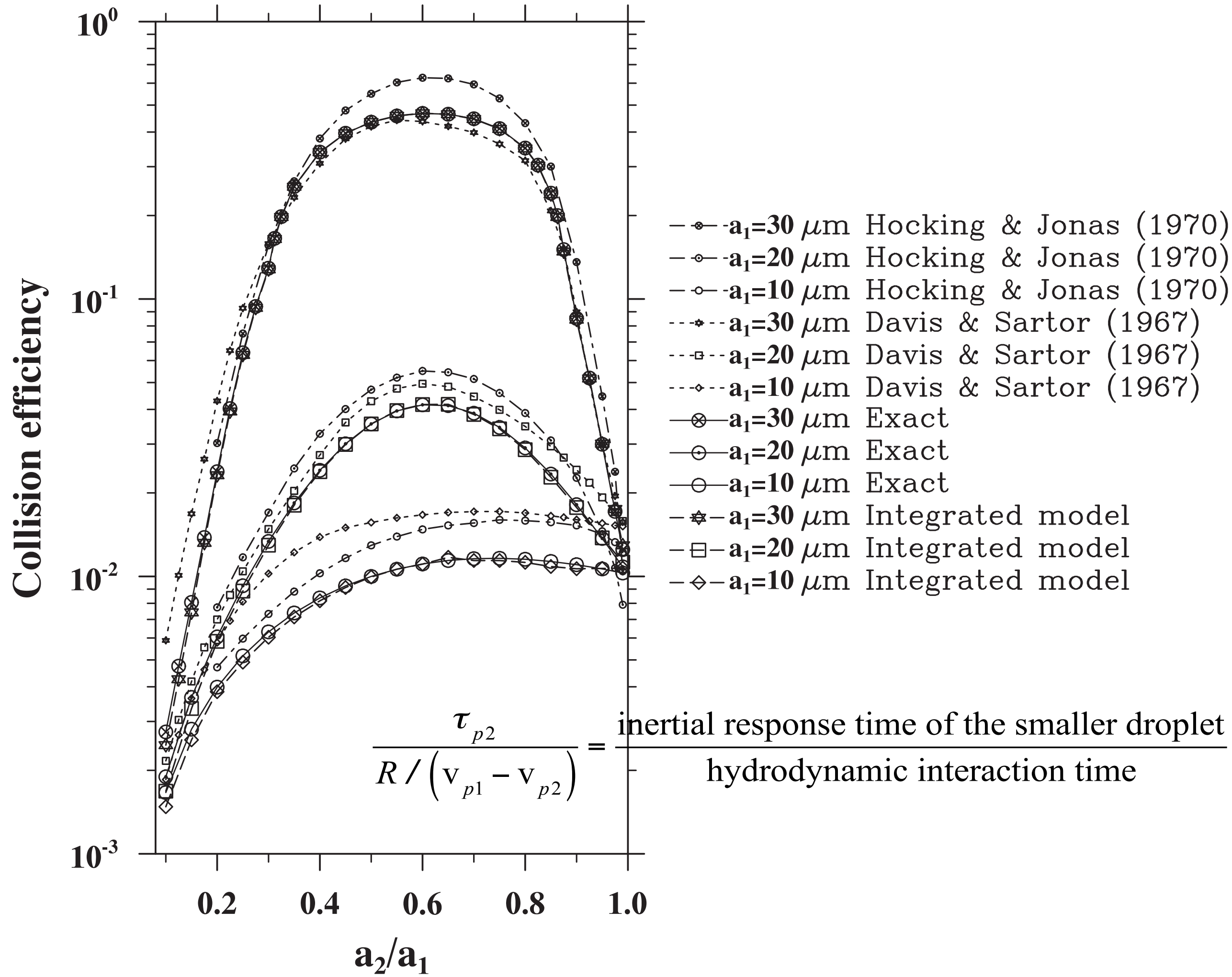
← Rosa et al. (2013), New J. Phys.

The collision efficiency

Local hydrodynamic interactions: gravitational collision efficiency



Rigorous collision efficiency in still air



$$\frac{\tau_{p2}}{R / \left(v_{p1} - v_{p2} \right)} = \frac{\text{inertial response time of the smaller droplet}}{\text{hydrodynamic interaction time}}$$

Rosa, Wang, Maxey, and Grabowski, 2011, An accurate model for aerodynamic interactions of cloud droplets, J. Comp. Phys., 230, 8109-8133.

Back of the envelope analysis

a_1	$\frac{a_2}{a_1}$	τ_{p2} (s)	$W_{1,Stokes}$ (cm/s)	$W_{2,Stokes}$ (cm/s)	$\frac{10R}{\Delta W_{Stokes}}$	$\frac{\tau_{p2}}{10R/\Delta W_{Stokes}}$	E (Stokes, gravity)
$30\mu m$	0.20	4.48×10^{-4}	10.963	0.4385	3.42×10^{-3}	0.131	0.04566
$30\mu m$	0.50	2.80×10^{-3}	10.963	2.7407	5.47×10^{-3}	0.512	0.5273
$30\mu m$	0.90	9.06×10^{-3}	10.963	8.8800	2.74×10^{-3}	0.330	0.1875

$$E \sim \left(\frac{\tau_{p2}}{10R/\Delta W_{Stokes}}\right)^{1.85}$$

$$\tau_p = \frac{2}{9}\left(\frac{\rho_p}{\rho_f}-1\right)\frac{a^2}{\upsilon}$$

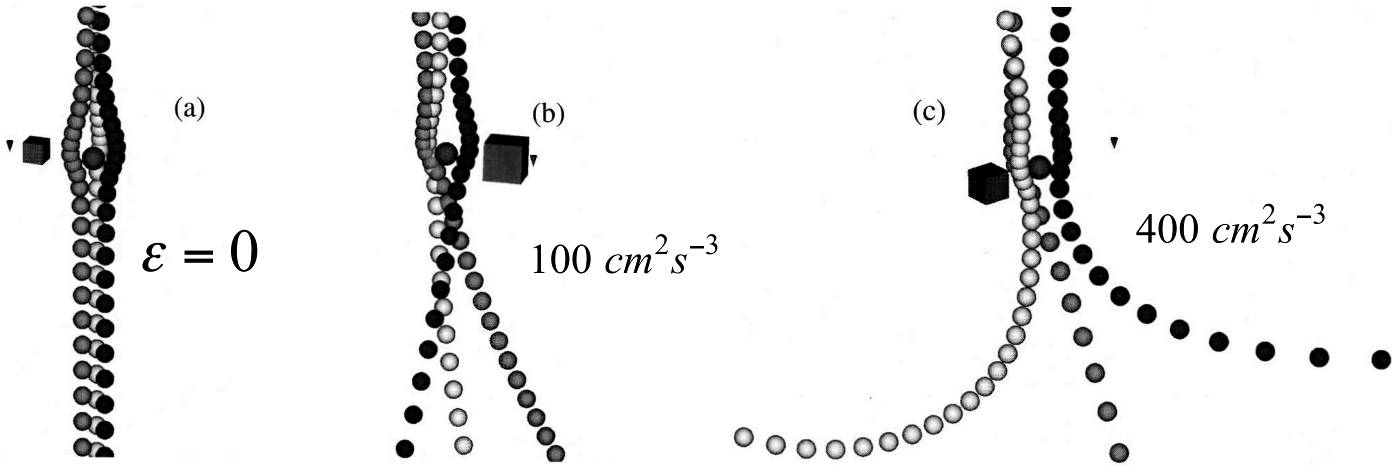
$$W_{Stokes} = \tau_p g$$

The collision efficiency
based on point-droplet hybrid DNS using ISM

How to obtain turbulent collision efficiency in point-droplet based DNS?

$$\eta_{12}^{T} \equiv \frac{E_{12}^{Turb}}{E_{12}^{g}}, \qquad E_{12}^{g} = \left[\frac{x_{grazing}}{(a_1 + a_2)}\right]^2, \qquad E_{12}^{Turb} = \frac{\Gamma_{12}^{Turb,\, HI}}{\Gamma_{12}^{Turb,\, No-HI}}$$

$$\text{where} \quad \Gamma_{12}^{HI} = \frac{\dot{N}^{Turb,HI}}{\langle n_1 \rangle \langle n_2 \rangle}, \qquad \Gamma_{12}^{Turb,\, No-HI} = \frac{\dot{N}^{Turb,\, No-HI}}{\langle n_1 \rangle \langle n_2 \rangle}$$



Three grazing trajectories of 20-μm droplets relative to 25-μm droplets

$dt = 0.42\tau_p(20\mu m)$

Wang, *et al.*, J. Atmos. Sci. 62: 2433-2450 (2006).
Ayala *et al.*, J. Comp. Phys. 225: 51-73. 62 (2007).

Does turbulent air flow enhance collision efficiency? By how much?

TABLE 1. Collision efficiencies in turbulent flow: previous formulations and results.

	de Almeida (1976, 1979)	Grover and Pruppacher (1985)	Kozoil and Leighton (1996)	Pinsky et al. (1999)
E_{12}	$\frac{2}{R^2}\int_0^\infty yP(y)\,dy$	$\langle\Gamma_{12}\rangle/(\pi R^2 v_d)$	$\frac{R_0^2}{R^2}\int_0^\pi P(\theta; R_0)\sin(2\theta)\,d\theta$	$\langle S_c\rangle/(\pi R^2)$
(a_1, a_2) (μm)	(25, 10 → 20)	(40→100, 1→5)	(10 → 20, 2 → 19)	(10 → 30, 1 → 29)
ϵ ($cm^2\ s^{-3}$)	10	100	100	100
E_{12}/E_{12}^g	3.40 → 5.49	Up to 100	≤1.60	2.0 → 4.0
HI model	Klett and Davis (1973)	Numerical flow	Stokes flow	Stokes flow
Turbulence	2D eddy flow	1D eddy flow	3D random field	3D random field

Wang et al. (2005 – 2009)

E_{12}^{Turb}: $\dfrac{\Gamma_{12}^{Turb,\,HI}}{\Gamma_{12}^{Turb,\,No-HI}}$

(a_1, a_2) (μm): $10 \sim 60\ \mu m$

ε : $100,\ 400\ cm^2 s^{-3}$

$E_{12}^{Turb} / E_{12}^{g}$: could be up to 4 (but mostly 1 to 2)

HI model: Improved superposition

Turbulence: DNS

Chen et al. (2018)

E_{12}^{Turb}: $\dfrac{\Gamma_{12}^{Turb,\,HI}}{\Gamma_{12}^{Turb,\,No-HI}}$

(a_1, a_2) (μm): $5 \sim 25\ \mu m$

ε : $20 \sim 500\ cm^2 s^{-3}$

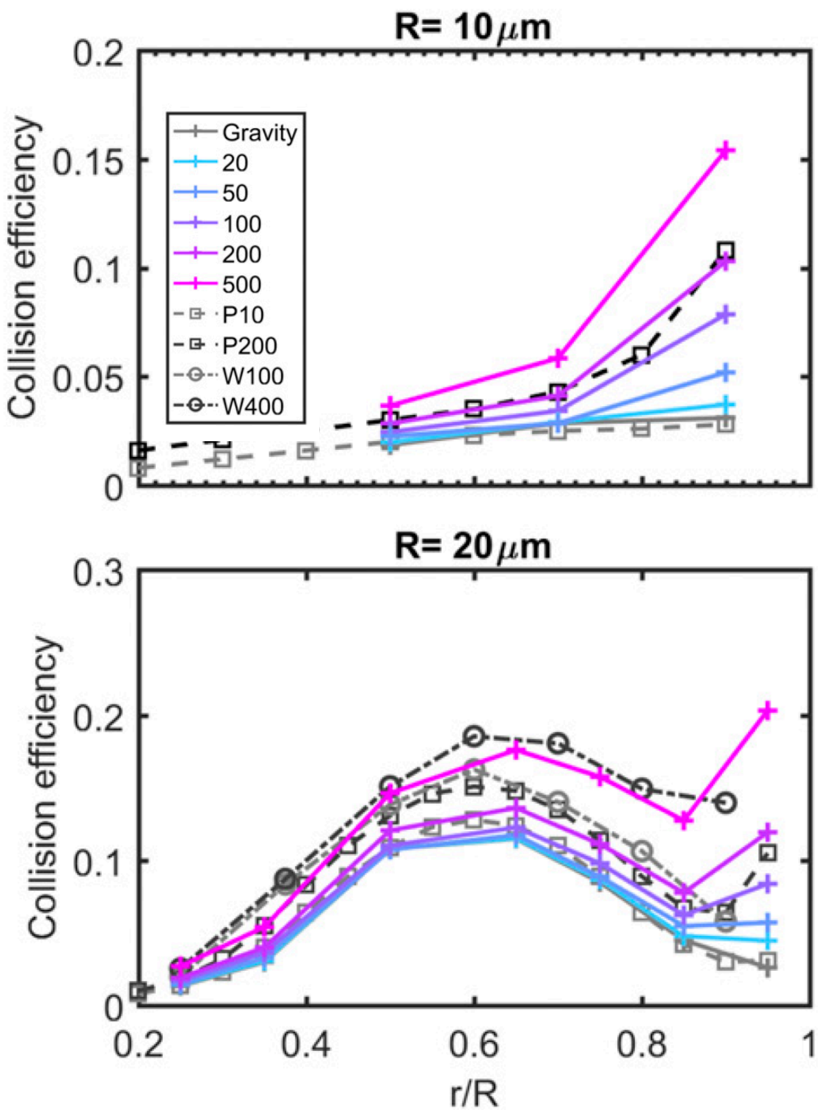
$E_{12}^{Turb} / E_{12}^{g}$: could be up to 6 (but mostly 1 to 2)

HI model: Improved superposition

Turbulence: DNS

Wang et al., New J. Phys. 10: 075013 (2008); Atmos. Sci. Lett. 10: 1–8 (2009).
Chen et al., J. Atmos. Sci., 2018.

Comparison of turbulent collision efficiencies from the ISM



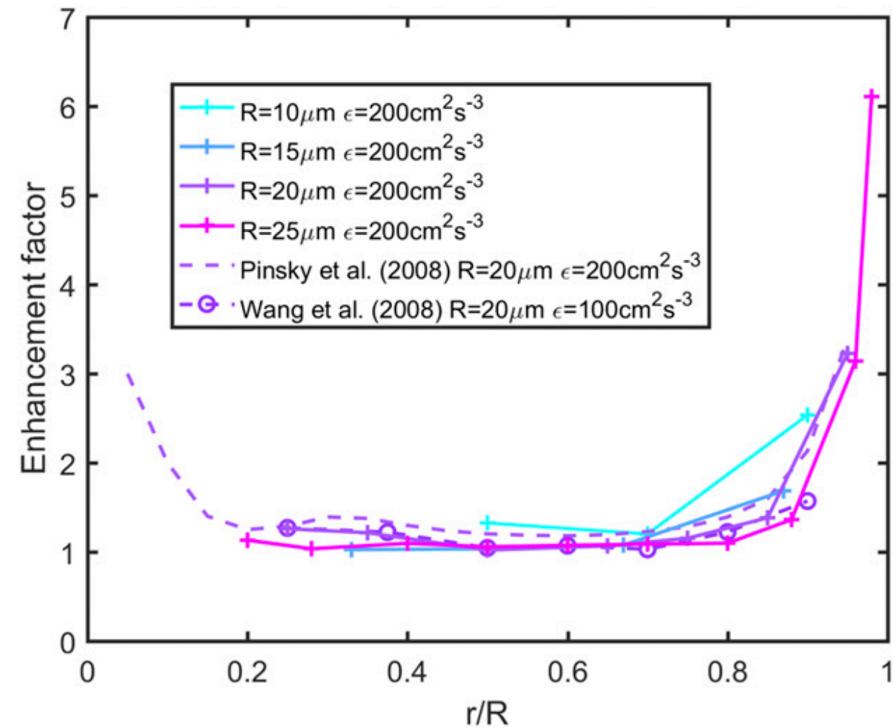


FIG. 3. Turbulence enhancement factor of collision efficiency for all four collector droplets at a dissipation rate of 200 $cm^2 s^{-3}$ (solid lines with cross markers). Enhancement factor of $R = 20\ \mu m$ from Wang et al. (2008) at $\varepsilon = 100\ cm^2 s^{-3}$ with Reynolds number of 72.4 and from Pinsky et al. (2008) at $\varepsilon = 200\ cm^2 s^{-3}$ are shown for comparison.

Chen, Yau, Bartello, J. Atmos. Sci., 2018.

General kinematic collision kernel: Finite-inertia droplets in a turbulent flow

Turbulent collision efficiency

$$\Gamma_{12} = \frac{\dot{N}}{\langle n_1 \rangle \langle n_2 \rangle} = 2\pi\, R^2 \langle |\, w_r(r=R)\,| \rangle g_{12}(r=R) \cdot \eta_{12}^T$$

Geometric Radial relative velocity

Geometric radial distribution function

$$\langle |\, w_r \,| \rangle = \frac{1}{N_{pair}} \sum_{all\ pairs} \left| \vec{r} \cdot \frac{(\vec{V}_1 - \vec{V}_2)}{r} \right|$$

$$g_{12}(R) = \lim_{\delta << r} \frac{N_{pair}(r-\delta \le d \le r+\delta)/4\pi\left[(r+\delta)^3 - (r-\delta)^3\right]}{N_1 N_2 / V_B}$$

- Non-overlap corrections when hydrodynamic interactions are considered

Important for parameterization of collection kernel.

Sundaram & Collins, J. Fluid Mech. 335: 75-109 (1997).
Wang, *et al.* J. Atmos. Sci. 62: 2433-2450 (2005).

Acceleration of the calculation of disturbance flows

$$\vec{u}^{(k)} = \vec{U}(\vec{x},t) + \sum_{\substack{m=1 \\ m\neq k}}^{N_p} \vec{u}_s\left(\vec{Y}^{(k)} - \vec{Y}^{(m)}; a^{(m)}, \vec{V}^{(m)} - \vec{U}\left(\vec{Y}^{(m)},t\right) - \vec{u}^{(m)}\right)$$

Gauss-Seidel iteration → GMRes (generalized minimal residual) with preconditioner

60% ~ 70% → less than 10%

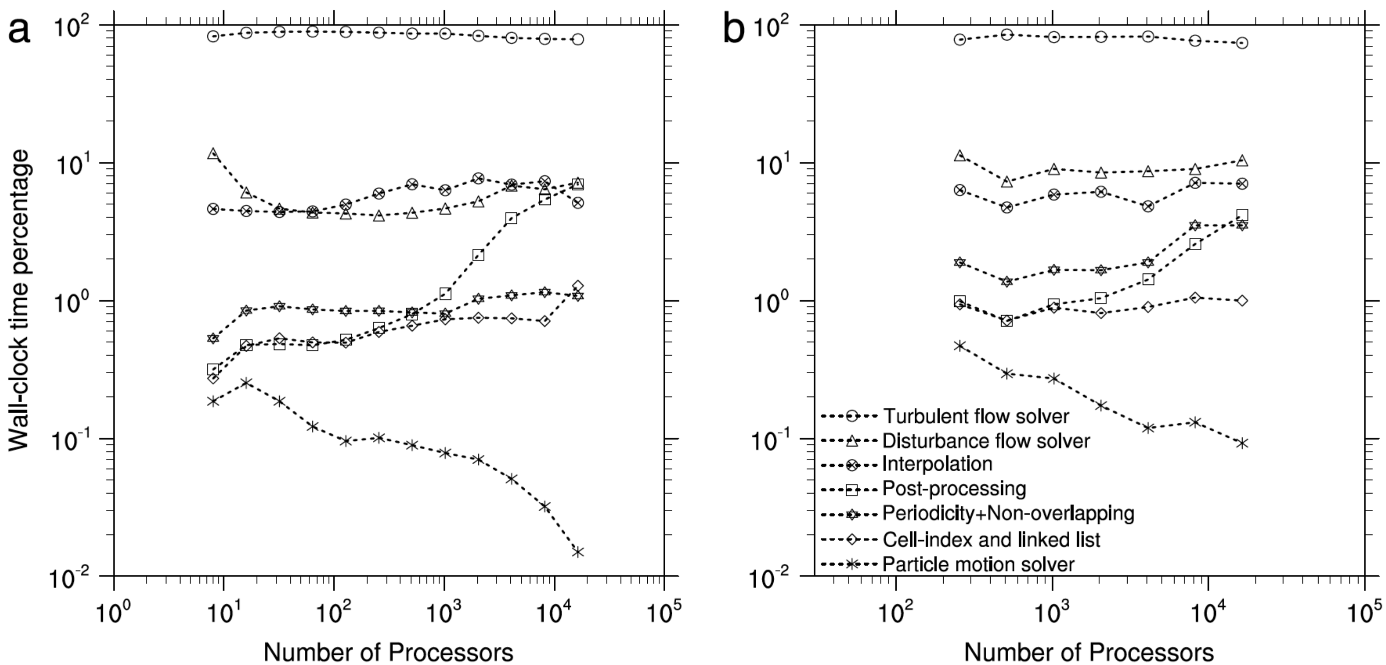


Fig. 4. Relative percentages of the wall-clock time spent on each subroutine for two cloud microphysics parameter settings: (a) 512^3, 45–50 μm, 730,000 particles (LWC ~2.2 g/m^3), (b) 1024^3, 20–30 μm, 16,500,000 particles (LWC ~ 1.0 g/m^3). Here LWC indicates the liquid water content.

Or approximate as pairwise sum assuming the volume fraction is very low (Onishi et al. 2013)

Torres et al., J. Comp. Phys. 245 (2013) 235-258.
Ayala et al., Computer Physics Communications 185 (2014) 3269–3290.
Onishi et al. , J. Comp. Phys. 242 (2013) 809-827.

Problem with the improved superposition method

Two main issues:

(1) Stokes disturbance flows are assumed.

(2) The improved superposition method is not accurate for short-range interactions.

Rosa et al. (2011) developed an efficient model to correct this problem in ISM.

Open research:

- Incorporated this model in the hybrid DNS code;
- Gathering collision efficiency data

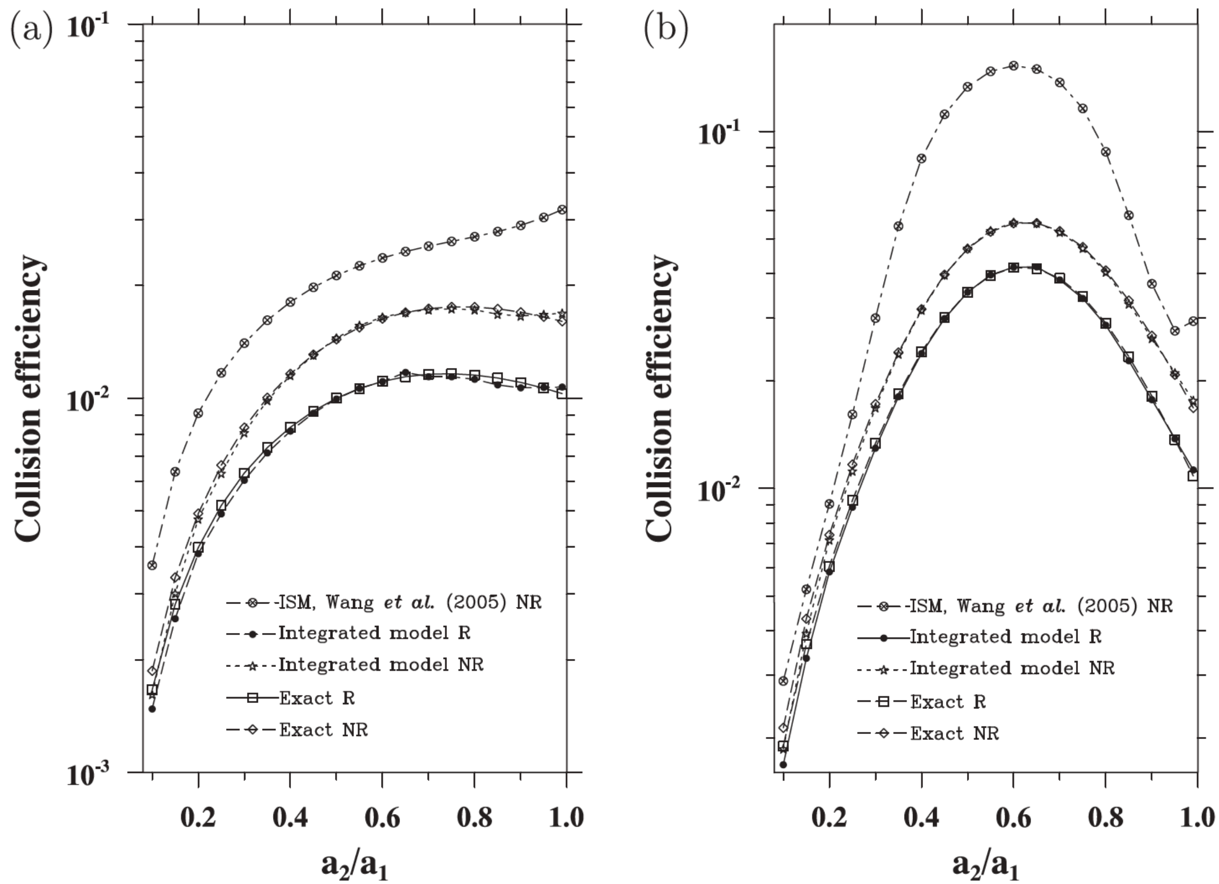


Fig. 13. A comparison of collision efficiency with previously published results. (a) a_1 = 10 μm; (b) a_1 = 20 μm.

Rosa, Wang, Maxey, Grabowski, An accurate and efficient method for treating aerodynamic interactions of cloud droplets, J. Comp. Phys. 230 (2011) 8109 – 8133.

Overview: Turbulent collision efficiency

$$E_{12}^{T} = E_{12}^{g} \times \frac{E_{12}^{T}}{E_{12}^{g}}$$

Gravitational collision efficiency

Enhancement factor by turbulence

Davis & Sartor (1967)

Klett & Davis (1973)

Davis (1984)

Jeffrey & Onishi (1984)

Pinsky et al. (1999,2007)

Wang et al. (2005, 2008)

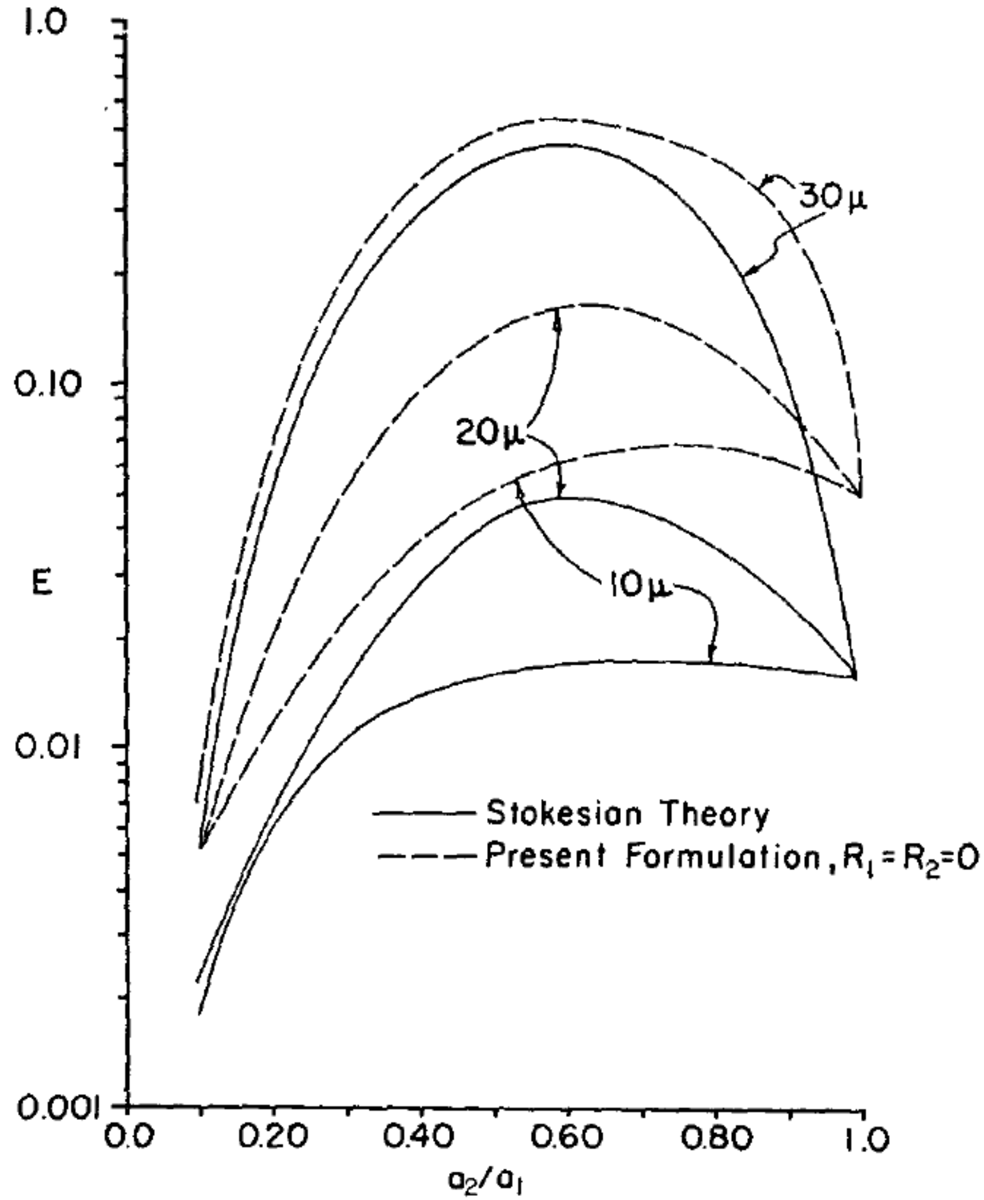
Chen et al. (2018)

Almost all studies assume Stokes disturbance flows

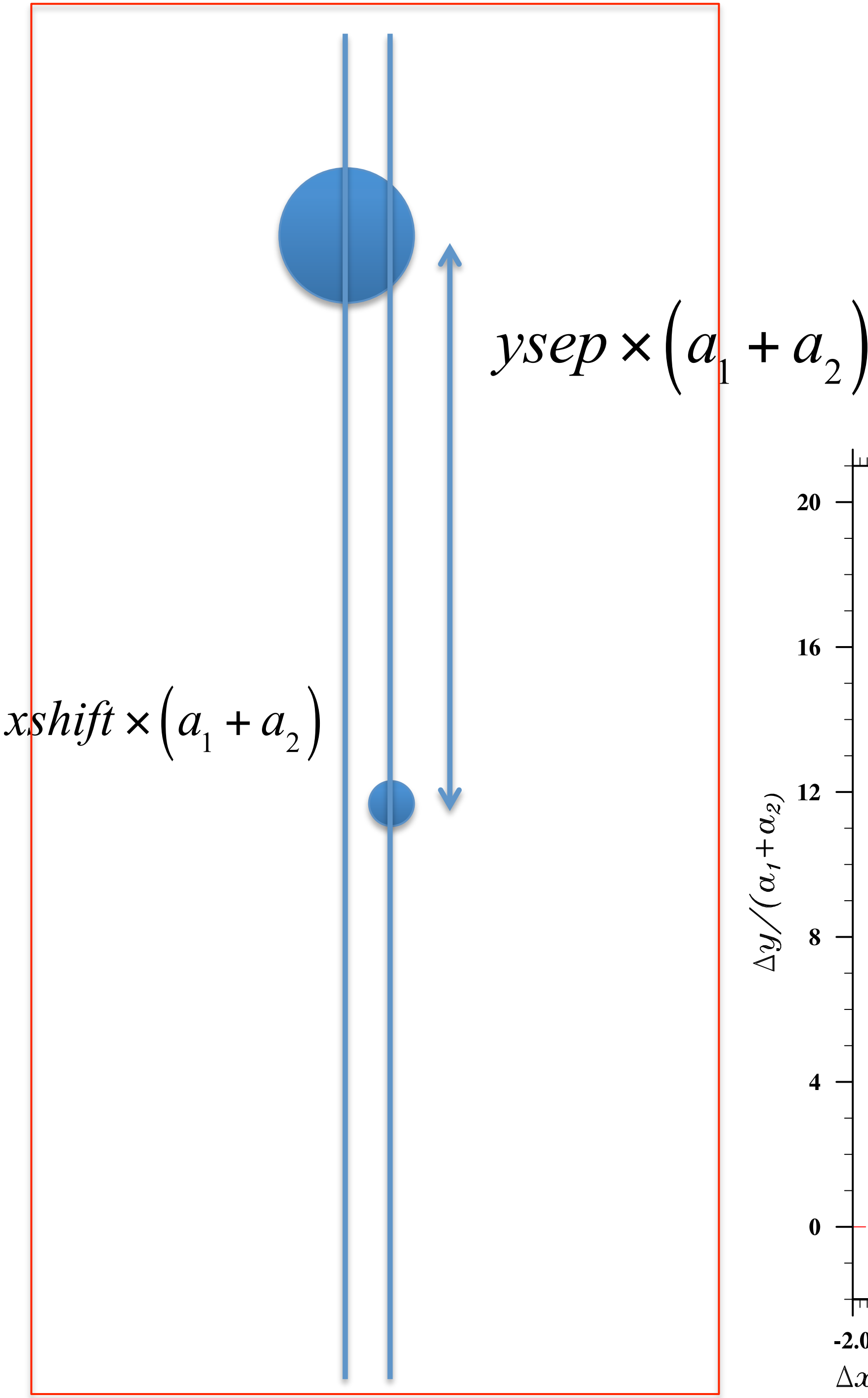
Finite-Re effect on collision efficiency: Deviations from Stokes flow are significant

Klett and Davis (1973)

They used Oseen flow correction to formulate the problem



The collision efficiency based on droplet-resolving DNS

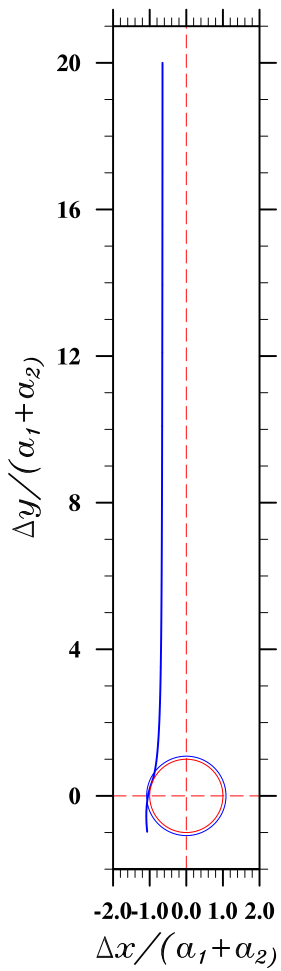


The problem description

$$No \;\; \text{HI:} \quad \pi (a_1 + a_2)^2$$

$$with \;\; \text{HI:} \quad \pi (xshift)^2 (a_1 + a_2)^2$$

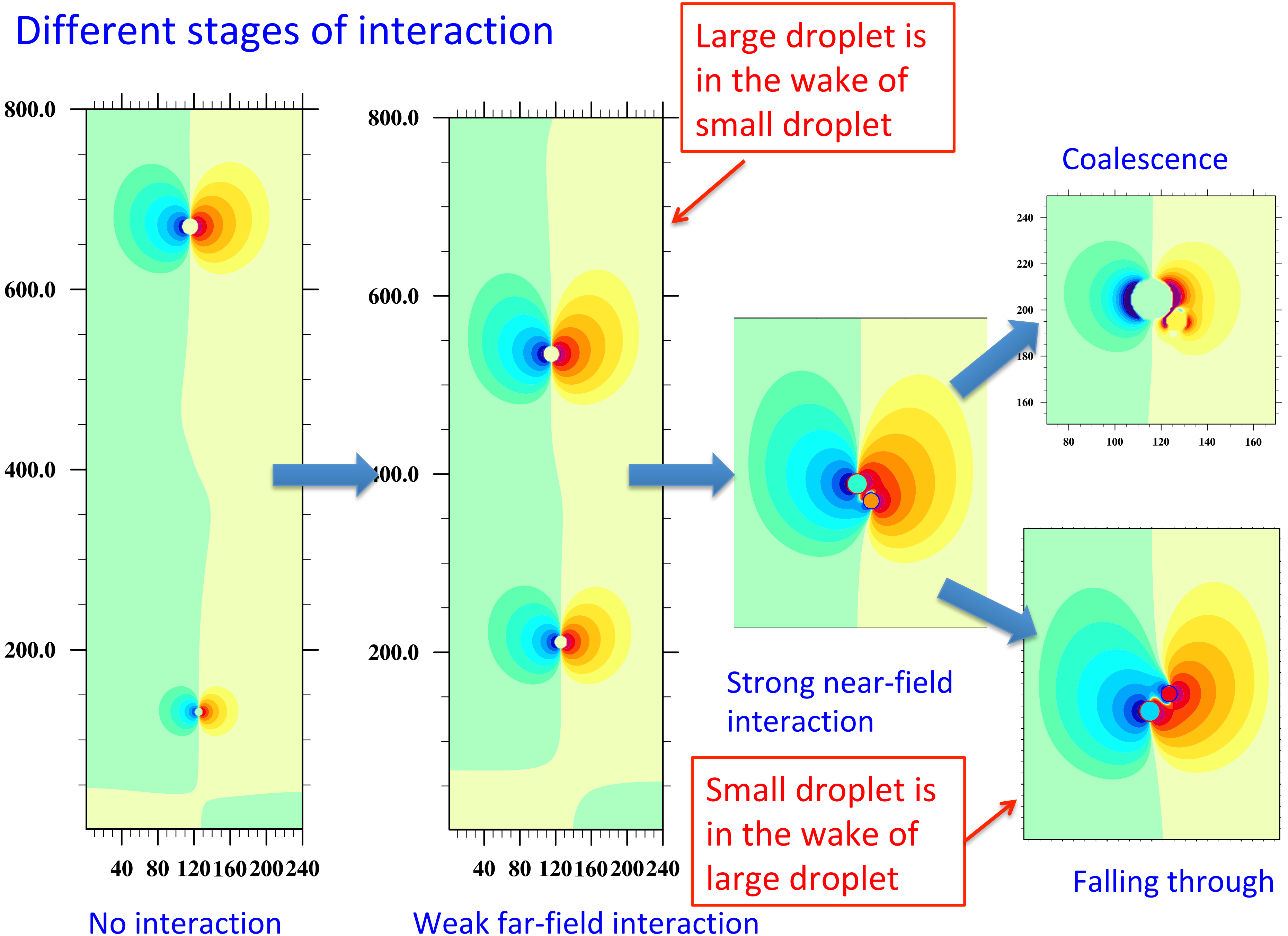
$$\eta = (xshift)^2$$



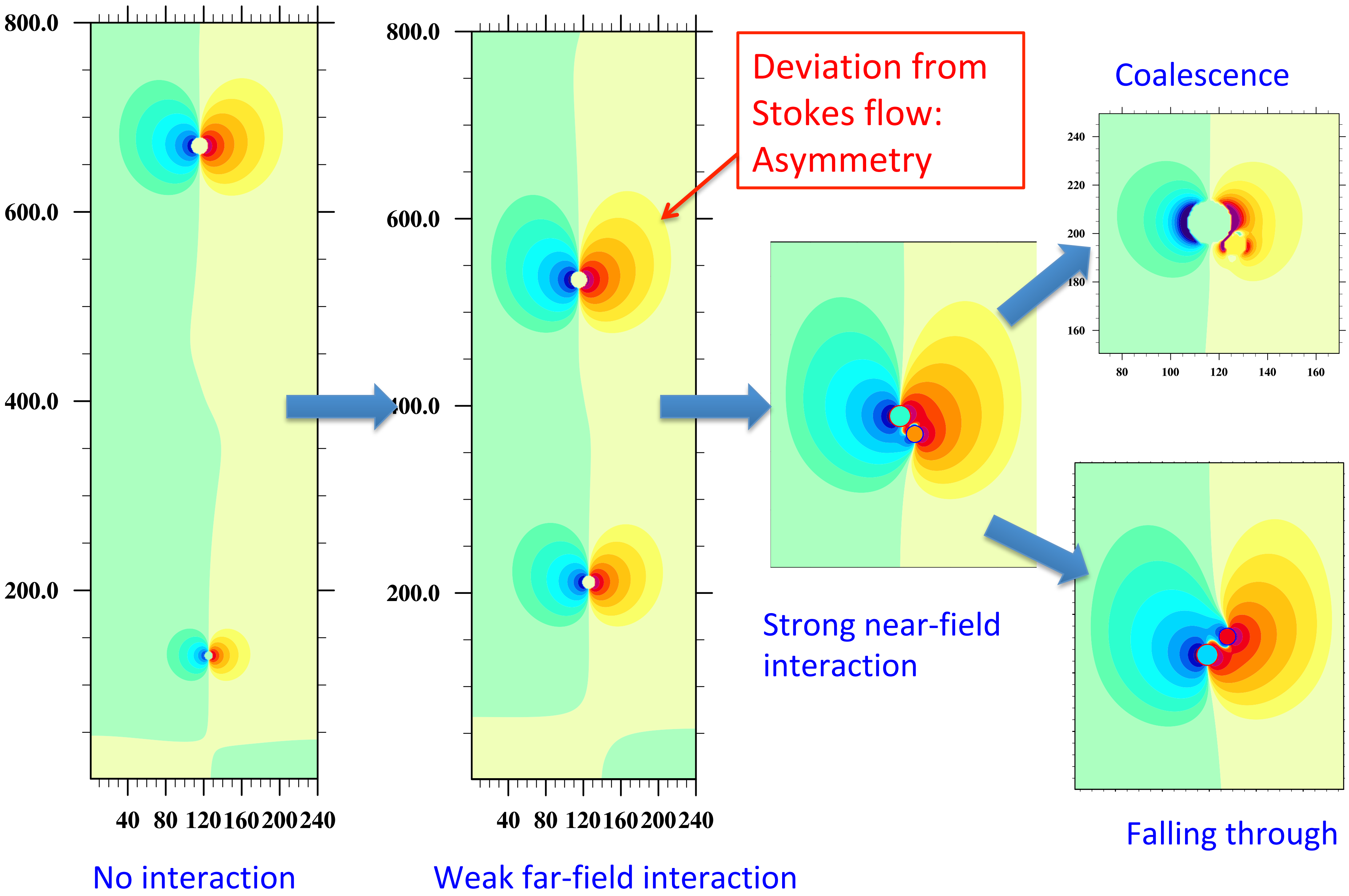
The goal is to find xshift for grazing trajectory

It is a multiscale problem!
Far-field interaction
Near-field interaction
Background flow field
(turbulent air)

Different stages of interaction



Different stages of interaction



The interface-resolved simulation method

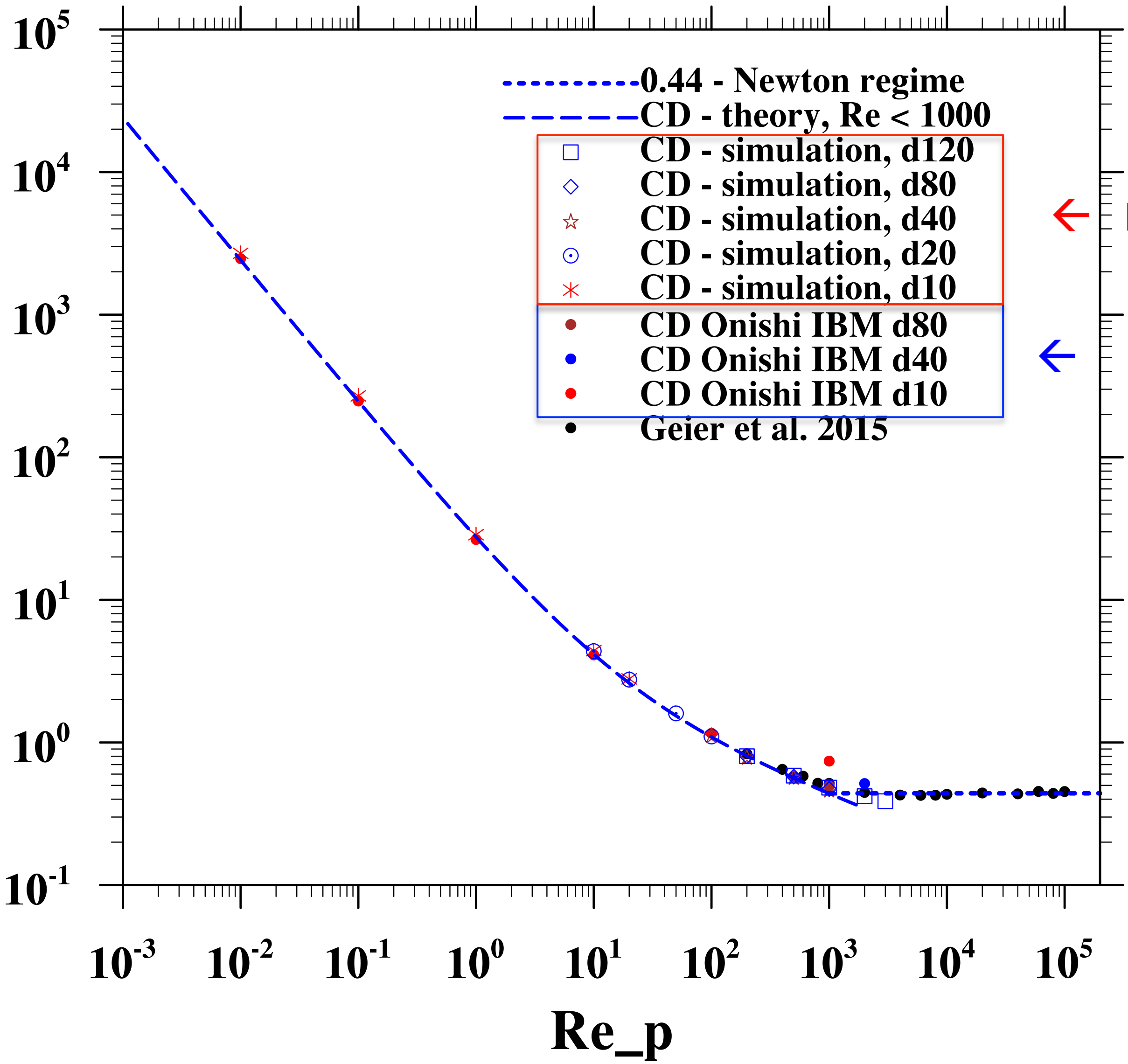
- ✧ Multiple-relaxation-time lattice-Boltzmann approach, D3Q19 (d'Humieres et al. 2002; Lallemand and Luo, 200)
- ✧ No flow inside solid particles
- ✧ No-slip boundary condition on the moving particle surface: 2nd-order interpolated bounce-back scheme

Not by IBM

- ✧ Direct momentum exchanges are used to compute interaction force and torque
- ✧ Nonuniform forcing implemented following Guo et al. (2002), Lu et al. (2012)
- ✧ Refill for new fluid nodes: constrained extrapolation
- ✧ Short-range particle-particle repulsion to prevent particle overlap (Glowinski et al. 2001; Feng and Michaelides 2005)
- ✧ MPI implementation based on 2D/3D domain decomposition

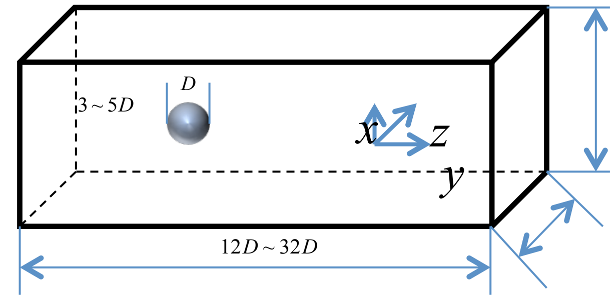
Peng et al., 2016, Implementation issues and benchmarking of lattice Boltzmann method for moving particle simulations in a viscous flow, *Comput. Math. Appl.*, 72: 349-374.

Drag coefficient as a function of Re_p



← LBM

← FD-IBM



$$C_D = \begin{cases} \frac{24}{Re_p}\left(1+0.15 Re_p^{0.687}\right) & Re_p < 1000 \\ 0.44, & Re_p \geq 1000 \end{cases}$$

Physical parameters

a_1	W_s(cm/s)	W(cm/s)	Re_p	$\tau_S(s)$
5	0.305	0.304	0.00203	0.000311
10	1.218	1.208	0.0161	0.00124
15	2.741	2.687	0.0537	0.00280
20	4.872	4.703	0.125	0.00497
25	7.613	7.207	0.240	0.00777
30	10.963	10.144	0.406	0.0112

Radius of the large particle is a_1

$a_1 = 30\ \mu m,\quad \text{vary } a_2 / a_1$

$g = 9.8\ \ \text{m/s}^2$

$\nu = 1.5\times 10^{-5}\quad \text{m}^2/\text{s}$

$\frac{\rho_p}{\rho_f} = 840$

Stokes terminal velocity

$$\text{w0} = \frac{2(\rho_p - \rho_f)a^2}{9\rho_f \nu} g$$

The more accurate terminal velocity

$$6\pi\rho_f \nu a W\left[1 + 0.15\left(\frac{2aW}{\nu}\right)^{0.687}\right] = \frac{4}{3}\pi a^3(\rho_p - \rho_f) g$$

Scale the problem with ρ_f, a_1, υ

time scale $= \frac{a_1^2}{\nu}$, length scale a_1, velocity scale $= \frac{\nu}{a_1}$

$\Rightarrow$ collision efficiency $= F\left(\frac{\rho_p}{\rho_f}, \frac{g a_1^3}{\nu^2}, \frac{a_2}{a_1},\right.$ domain size / exterier BCs, lubrication model parameters, coalescence criterion, ...$\left.\right)$

$$\frac{\text{w0} * a_1}{\nu} = \frac{2}{9}\left(\frac{\rho_p}{\rho_f} - 1\right)\left(\frac{a}{a_1}\right)^2 \frac{g a_1^3}{\nu^2}$$

$$Re_p = 2\left(\frac{a}{a_1}\right)\left(\frac{W * a_1}{\nu}\right)$$

$$\frac{\rho_p}{\rho_f} = 840,\quad \frac{g a_1^3}{\nu^2} = \frac{980\times 0.003^3}{0.15^2} = 0.001176,\quad \frac{a_2}{a_1} = \text{vary}$$

Lubrication interaction

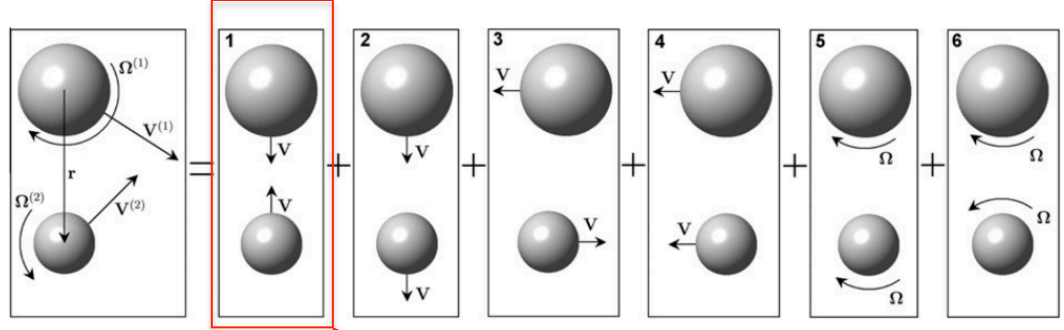


Fig. 1. Treating arbitrary two-body configuration by combining six simple interactions.

Correct for this for now

$$\lambda=\frac{a_2}{a_1} \quad \left(\text{note } a_2 < a_1\right),$$

normalized gap distance: $\varepsilon=\dfrac{2r}{\left(a_1+a_2\right)}-2=\dfrac{\left[r-\left(a_1+a_2\right)\right]}{\left(a_1+a_2\right)/2}$

$r =$ distance between the centers of the droplets

$$\frac{F_1}{6\pi\mu a_1 V}=c_{11}\frac{1}{\varepsilon}+c_{21}\ln\varepsilon+c_{31}*\varepsilon\ln\varepsilon+c_{41}$$

$$\frac{F_2}{6\pi\mu a_2 V}=c_{12}\frac{1}{\varepsilon}+c_{22}\ln\varepsilon+c_{32}*\varepsilon\ln\varepsilon+c_{42}$$

$$\vec{F}_{\text{lub},1}=3\pi\rho_0 \nu a_1\cdot\left(\vec{V}_1-\vec{V}_2\right)\cdot\frac{\vec{Y}_1-\vec{Y}_2}{\left|\vec{Y}_1-\vec{Y}_2\right|}\cdot\left[\tilde{F}_1\left(\varepsilon\right)-\tilde{F}_1\left(\varepsilon_0\right)\right]\times\frac{\vec{Y}_1-\vec{Y}_2}{\left|\vec{Y}_1-\vec{Y}_2\right|}$$

$$\vec{F}_{\text{lub},2}=-3\pi\rho_0 \nu a_2\cdot\left(\vec{V}_1-\vec{V}_2\right)\cdot\frac{\vec{Y}_1-\vec{Y}_2}{\left|\vec{Y}_1-\vec{Y}_2\right|}\cdot\left[\tilde{F}_2\left(\varepsilon\right)-\tilde{F}_2\left(\varepsilon_0\right)\right]\times\frac{\vec{Y}_1-\vec{Y}_2}{\left|\vec{Y}_1-\vec{Y}_2\right|}$$

$\tilde{F}_1\left(\varepsilon\right)$ is taken as the value in Table 3 of Rosa et al. (2011)

Rosa *et al.*, 2011, J. Comp. Phys.

Setting the gap distance to start lubrication-interaction correction

The lubrication correction is switched on when

$$\text{gap} \leq 0.125 \times \min\left[a_1, a_2\right]$$

$$\frac{a_2}{a_1} \rightarrow 1$$

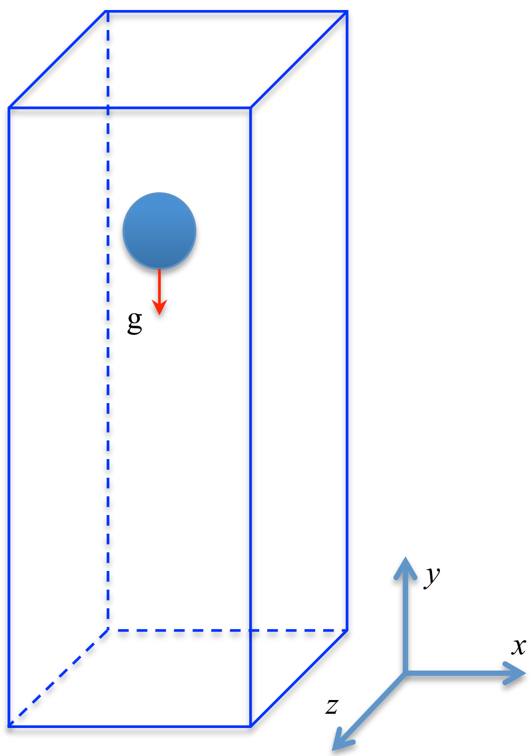
Should compare the total hydrodynamic force and the lubrication force at this gap distance?
The lubrication force should be dominating???

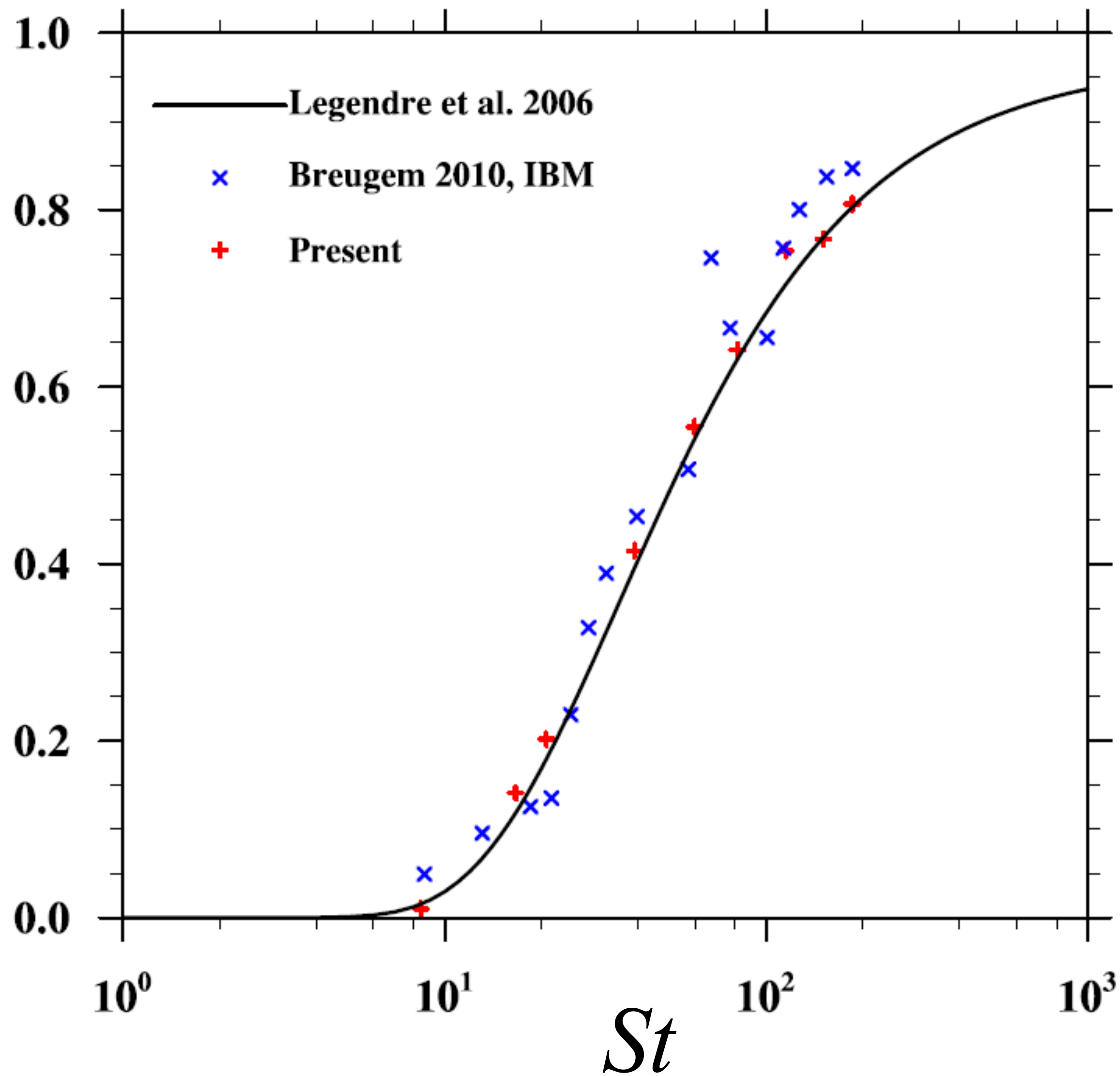
For two equal size particles, we find that 0.125 a is a good choice.

$$\frac{a_2}{a_1} \rightarrow 0$$

For particle-wall interaction. The wet coefficient of can be simulated by using $0.15a_2$.

Validation of lubrication correction treatment (plus soft sphere model): the wet coefficient of restitution





$$St = \frac{\tau_p}{a / W_{Stokes}} = \frac{\rho_p W_{Stokes} D}{9\mu_f},$$

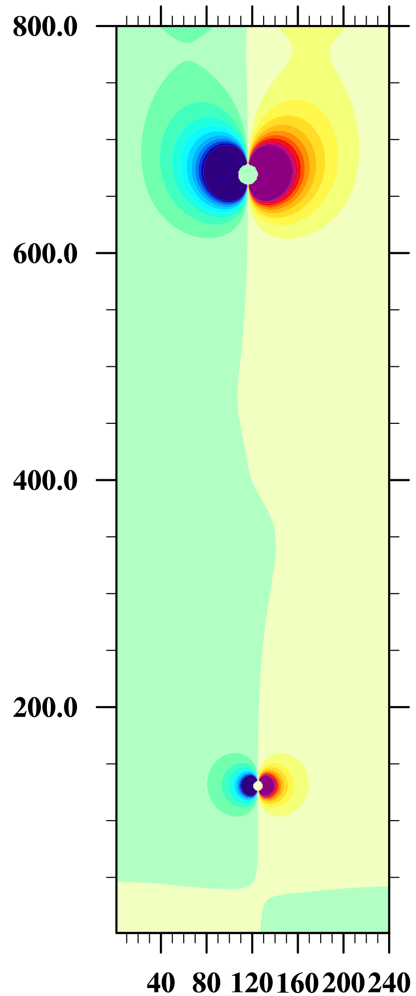
Domain size & boundary conditions

Domain size in lattice units:
240 by 800 by 200

a_1 = 9

Outlet

$$\left.\frac{\partial \rho_0 \vec{u}}{\partial t} + U \frac{\partial \rho_0 \vec{u}}{\partial y}\right|_{y=L_y} = 0$$



Side walls

$$w = 0, \frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = 0$$

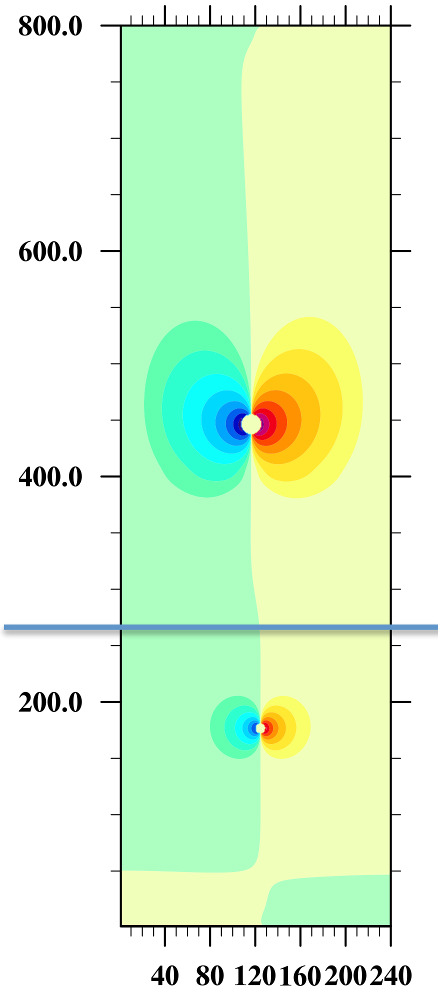
at $z = 0, z = L_z$.

Inlet

$$\vec{u}(y=0) = (0,0,0)$$

Designing direct numerical simulation: initialization

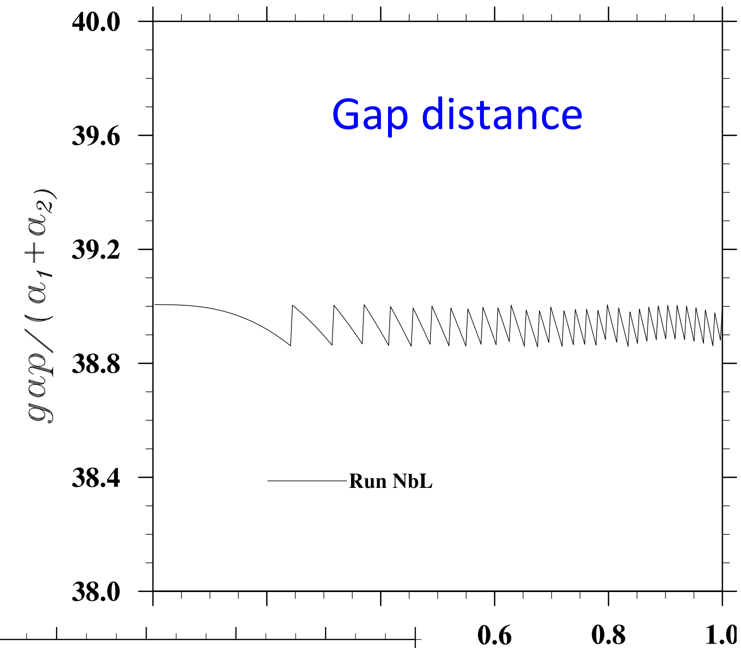
Stretching shift
+ Center shift

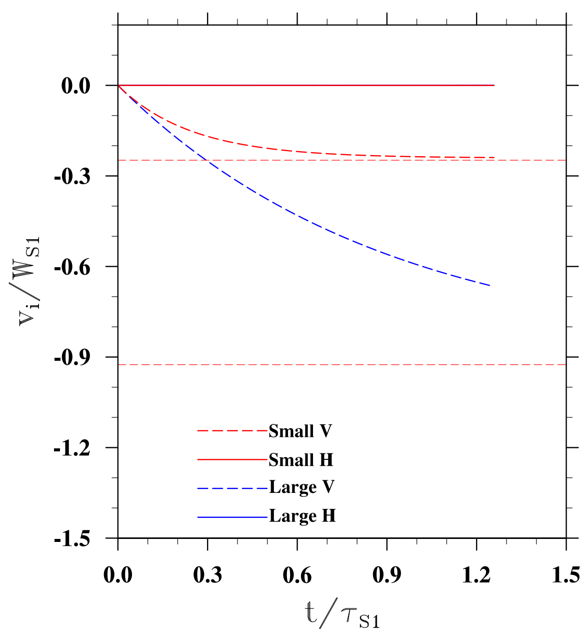


Shift
up

←two new
layers are added

Shift
down





Velocity is
smooth.

Fast initialization

$$\frac{dV}{dt} = -\frac{V}{\tau_S}\left(1+0.15\left(\frac{2a|V|}{\nu}\right)^{0.687}\right) - \left(1-\frac{\rho_f}{\rho_p}\right)g$$

We can accelerate the initial stage by

(1) reducing τ_S but

(2) keeping the terminal velocity constant

$$\tau_S = \frac{2\rho_p a^2}{9\rho_f \nu}, \qquad W_s = \frac{2\left(\frac{\rho_p}{\rho_f}-1\right)a^2}{9\nu}g$$

$$Faccel = 20 \text{ or } 10$$

For the initialization stage we can introduce a code-speed-up factor

$$[g] = g \times Faccel$$

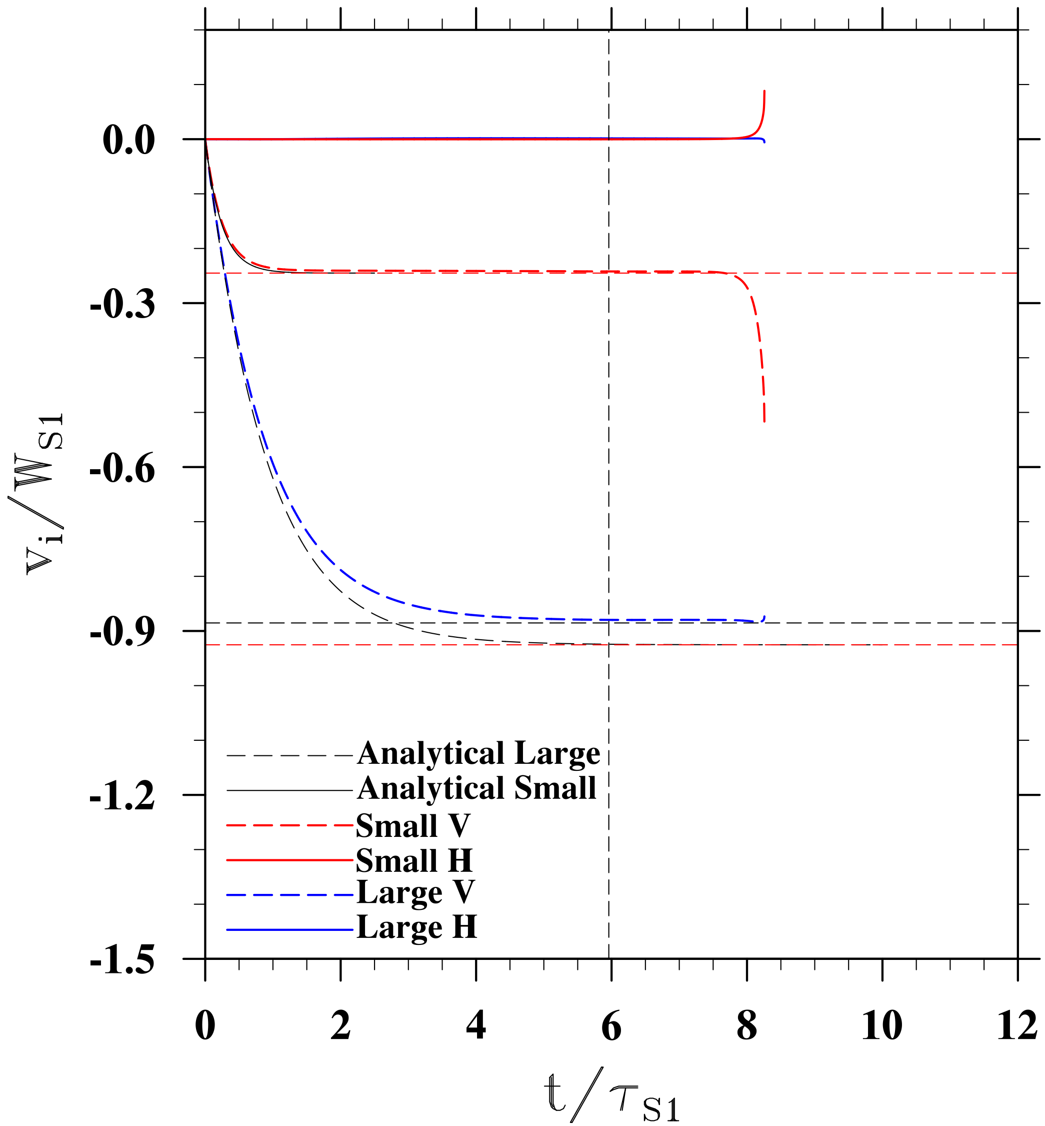
$$\left(\left[\frac{\rho_p}{\rho_f}\right]-1\right) = \left(\frac{\rho_p}{\rho_f}-1\right)\times\frac{1}{Faccel} \Rightarrow \left[\frac{\rho_p}{\rho_f}\right] = 1+\left(\frac{\rho_p}{\rho_f}-1\right)\times\frac{1}{Faccel}$$

The factor will be restored back to one after initialization.

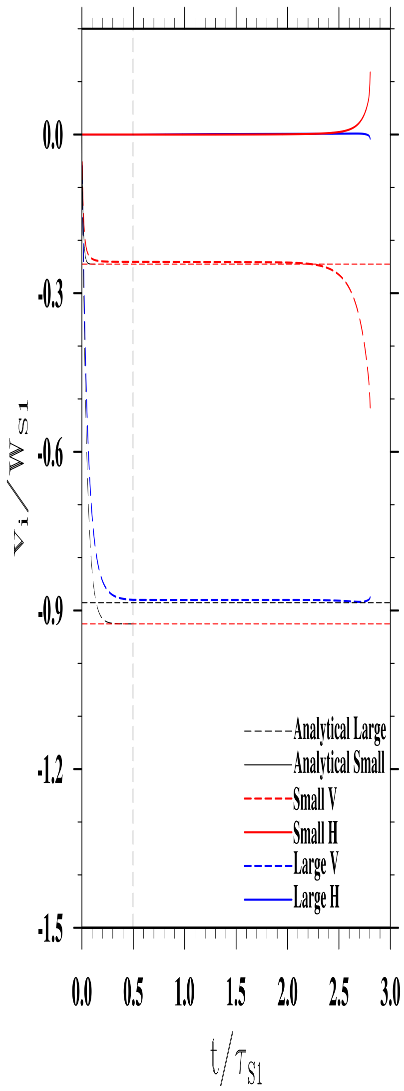
$$\text{rhopg} = \left(\frac{\rho_p}{\rho_f}-1\right) \text{g} \quad \text{remains fixed}$$

→ **Expect 20 or 10 times speed up!**

Typical evolution of droplet velocities



Before acceleration



After Acceleration

A typical set of simulations

$$\frac{a_2}{a_1} = 0.8$$

Run	x_shift	$\frac{d_{min} - (a_1 + a_2)}{(a_1 + a_2)}$	ysep	steps	
0.8*a*	0.600	coalescence	20	103,563	1 hr 38min
0.8*b*	0.650	coalescence	20	103,938	1 hr 38min
0.8*c*	0.750	falling through	20	118,353	1 hr 52min
0.8*d*	0.700	coalescence	20	104,416	
0.8*e*	0.725	falling through	20		
0.8*f*	0.7125	coalescence	20		

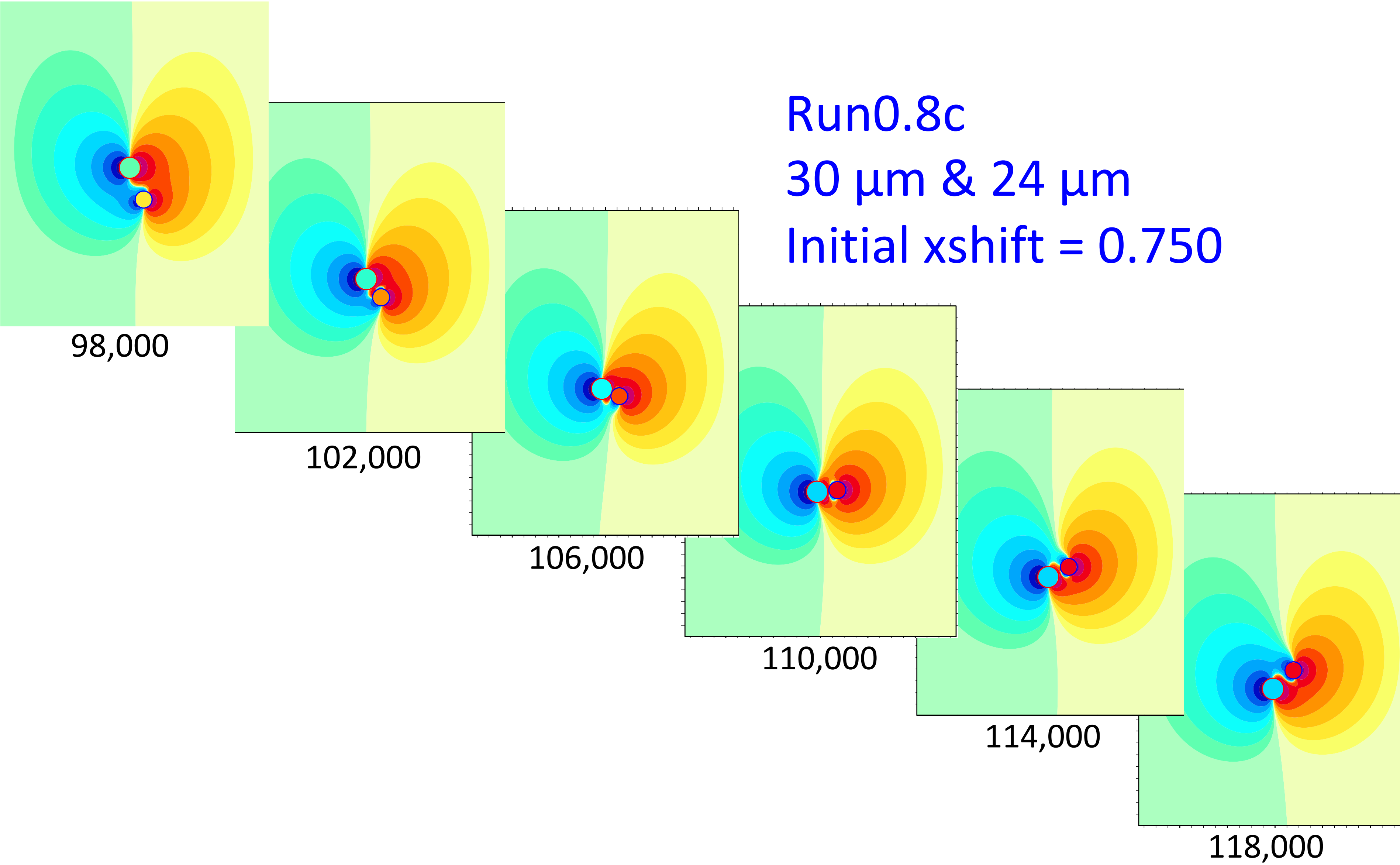
xshift = (0.725+0.7125)/2=0.71875

Faccel=20: 15,000 initialization

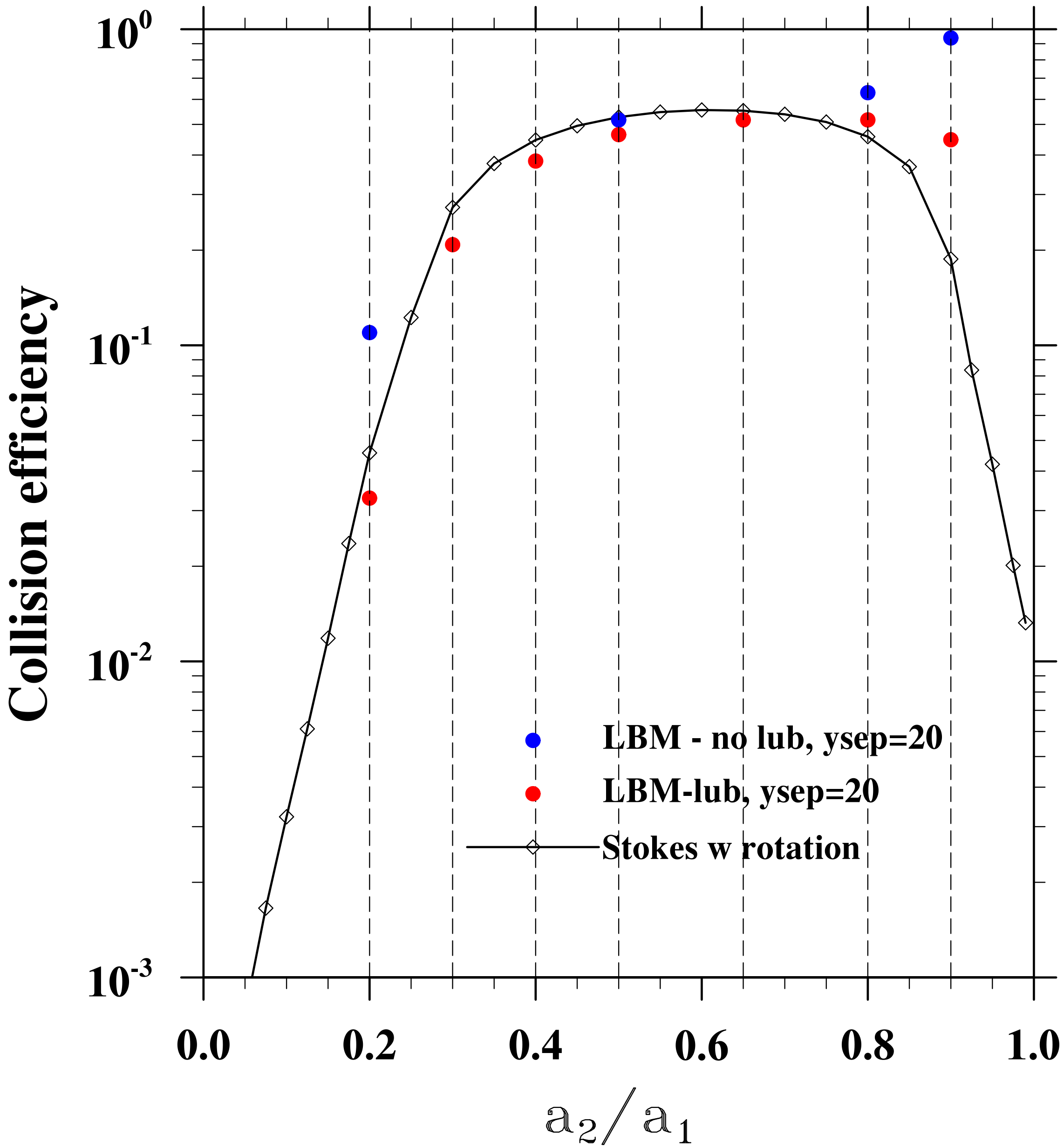
Run0.8c

30 µm & 24 µm

Initial xshift = 0.750



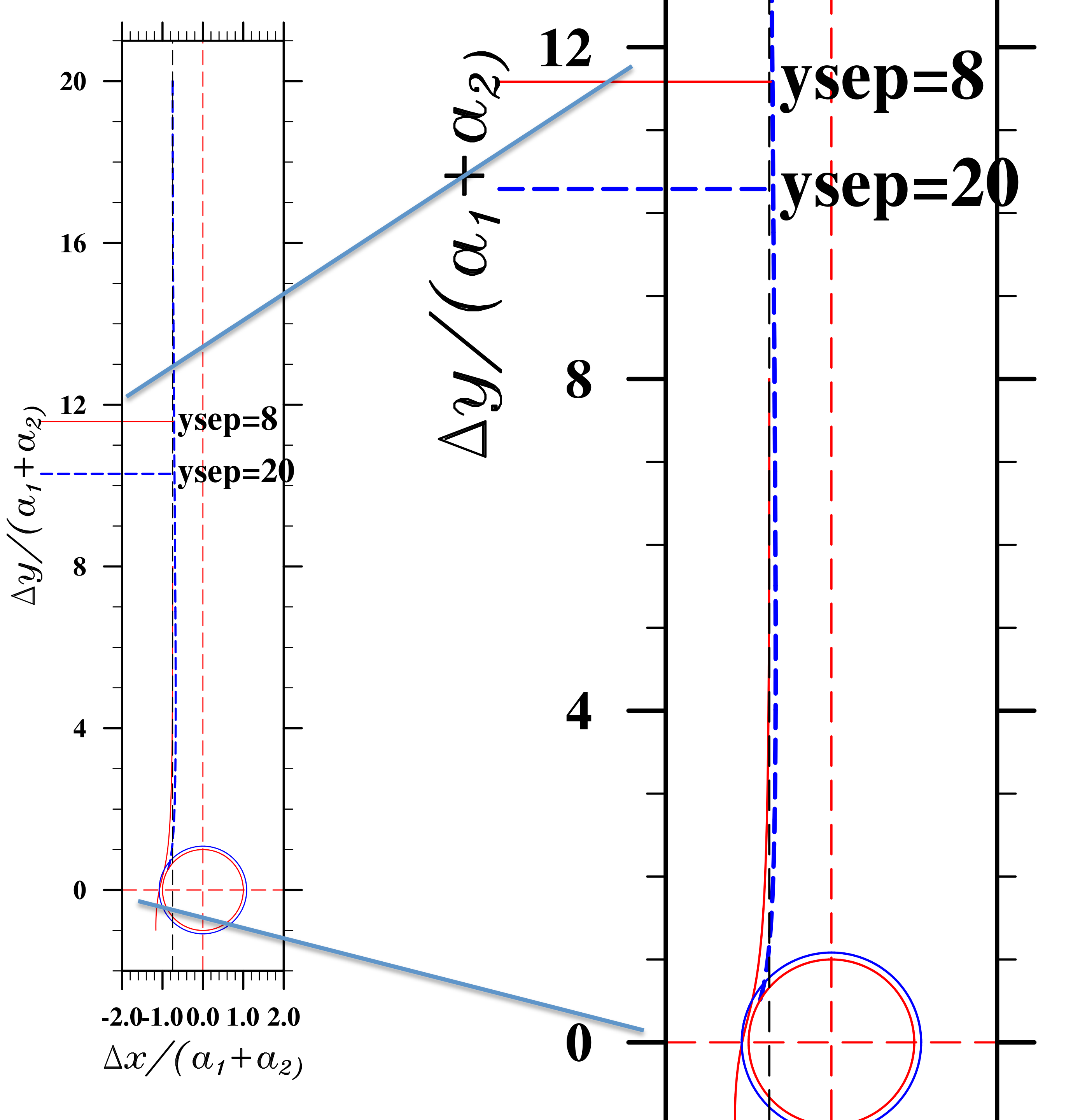
The effect of lubrication correction



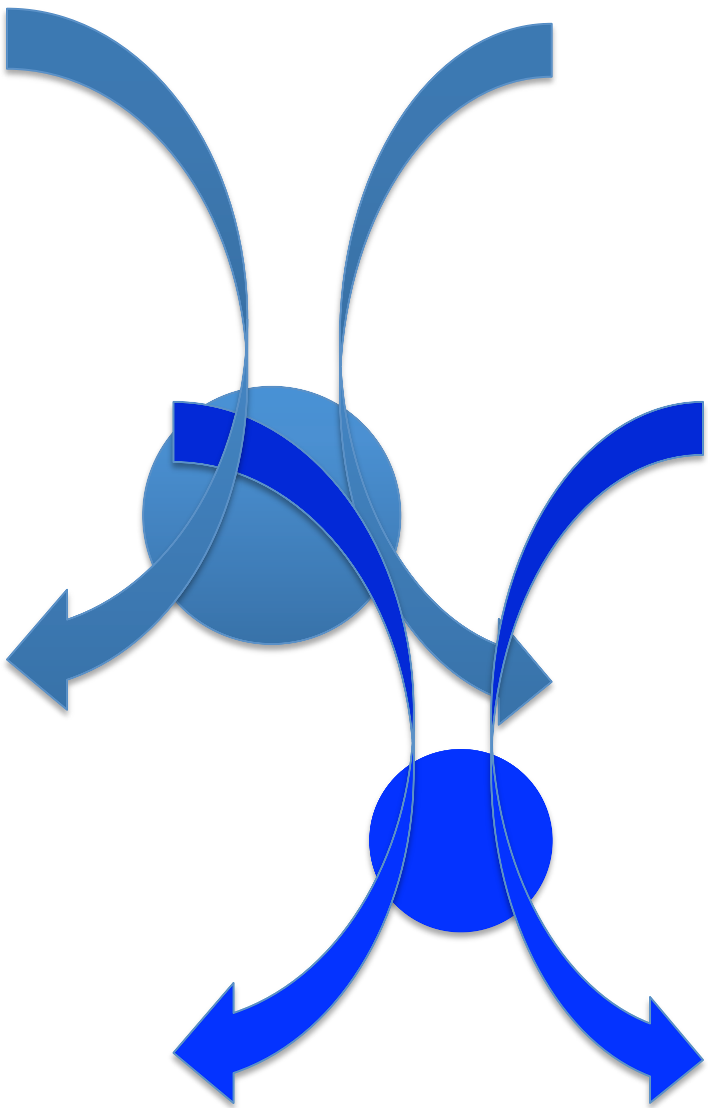
The Wake Effect

$$\frac{a_2}{a_1} = 0.80$$

$$xshift = 0.750$$

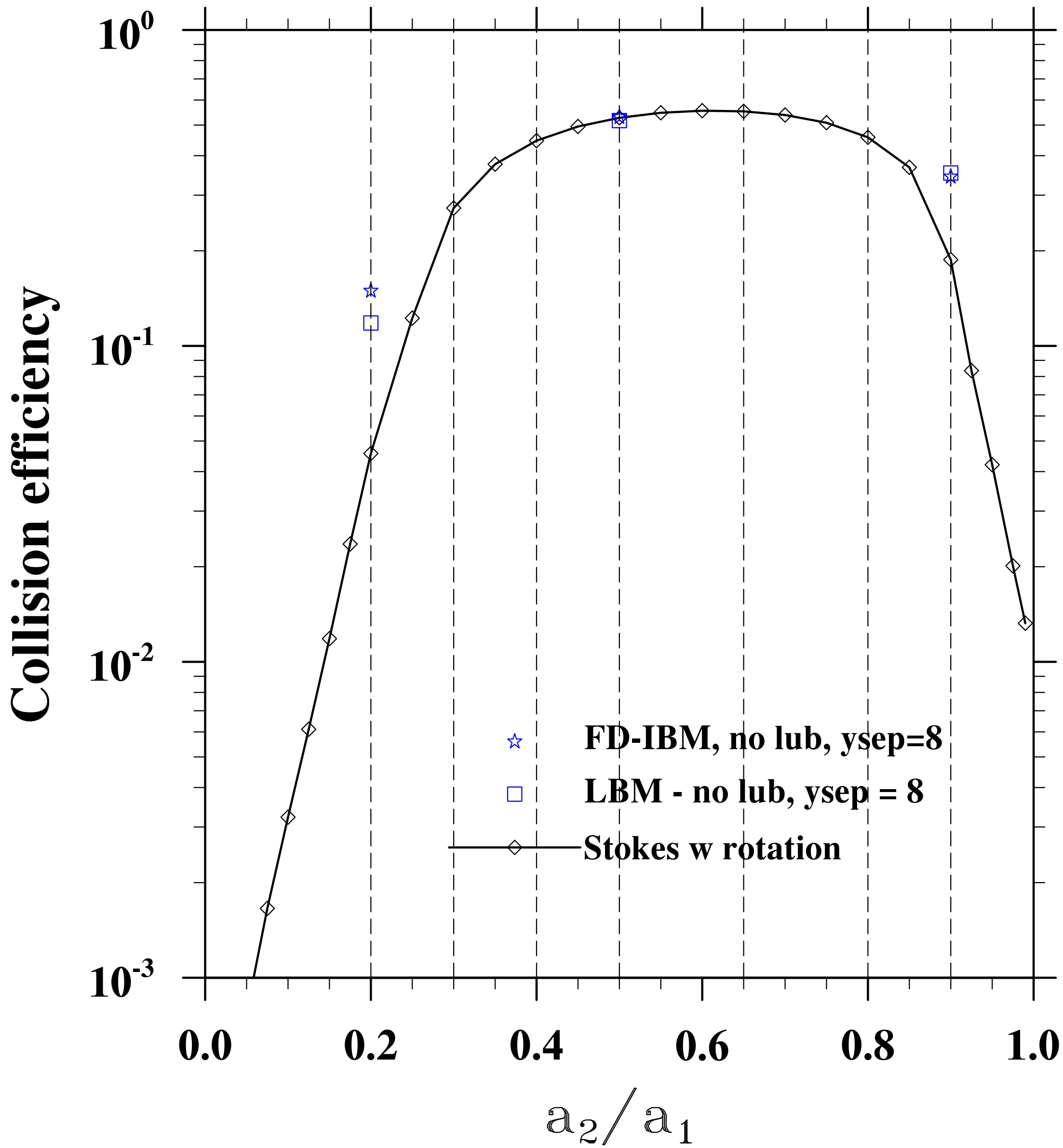


The wake effect sketch and conditions



- The wake of the small droplet has to be stronger than the front far-field disturbance flow of the large droplet
- This is possible due to (1) the asymmetry of the front and back (wake) flow; (2) the two droplets must be comparable in size. We can further investigate the disturbance flow to establish conditions for a2/a1 value and a1.

Comparison of two numerical methods



Discussions: The nonlinear drag effect

$\frac{a_2}{a_1}$	a_2 (μm)	$\tau_{p,Stokes}$ (s)	$(W_2)_{Stokes}$ (cm/s)	$(W_2)_{real}$ (cm/s)	$\frac{(W_2)_{real}}{(W_2)_{Stokes}}$	$Re_{p2,real}$	$\frac{(W_1-W_2)_{real}}{(W_1-W_2)_{Stokes}}$
0.20	6	0.0004475	0.4385	0.4372	0.997	0.00350	0.922 (-7.8%)
0.30	9	0.001007	0.9867	0.9797	0.993	0.0118	0.919 (-8.1%)
0.40	12	0.001790	1.7541	1.7320	0.987	0.0277	0.913 (-8.7%)
0.50	15	0.00280	2.7407	2.6867	0.980	0.0537	0.907 (-9.3%)
0.65	19.5	0.00473	4.6318	4.4785	0.967	0.116	0.895 (-10.5%)
0.80	24	0.00716	7.0163	6.6700	0.951	0.213	0.880 (-12.0%)
0.90	27	0.00906	8.8800	8.3333	0.938	0.300	0.869 (-13.1%)
1.00	30	0.01119	10.963	10.144	0.925	0.406	

$$\left[\frac{(W_1-W_2)_{real}}{(W_1-W_2)_{Stokes}}\right]^{1.85} = 0.861 \rightarrow 0.771$$
$$= 13.9\% \rightarrow 22.9\%$$

Is the nonlinear drag effect important?

First effect of deviation from Stokes flow.

Finite simulation domain size tends to attenuate the terminal velocity

$\frac{a_2}{a_1}$	a_2 (μm)	$(W_2)_{real}$ (cm/s)	$(W_2)_{simulated}$ (cm/s)	$\frac{(W_2)_{simulated}}{(W_2)_{real}}$	$\frac{(W_1 - W_2)_{simulated}}{(W_1 - W_2)_{real}}$
0.20	6	0.4372	0.4680	1.070	0.945 (-5.5%)
0.30	9	0.9797	1.0134	1.034	0.941 (-5.9%)
0.40	12	1.7320	1.7415	1.005	0.939 (-6.1%)
0.50	15	2.6867	2.6460	0.985	0.937 (-6.3%)
0.65	19.5	4.4785	4.3305	0.967	0.937 (-6.3%)
0.80	24	6.6700	6.3875	0.958	0.935 (-6.5%)
0.90	27	8.3333	7.9425	0.953	0.935 (-6.5%)
1.00	30	10.144	9.6363	0.950	

Far-field effect from the large droplet (rows 0.20–0.40)

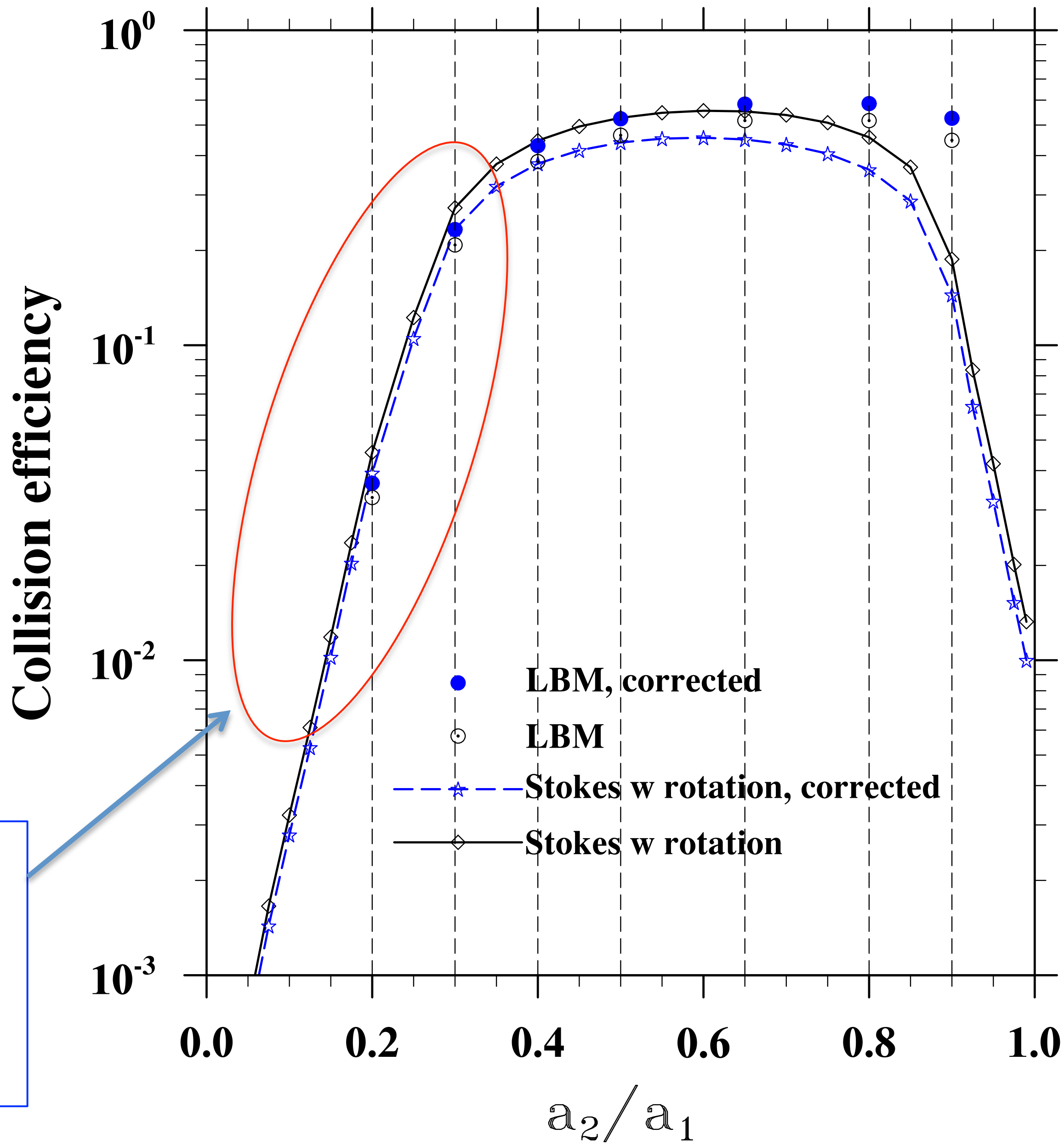
Domain size effect (rows 0.50–1.00)

$$W_{S,LBM}(a_1) = 1.21810 \times 10^{-2}$$
$$W_{S,Phys}(a_1) = 10.963 = 900 \times W_{S,LBM}(a_1)$$

Comparison: corrected collision efficiency vs corrected Stokes-disturbance-flow results

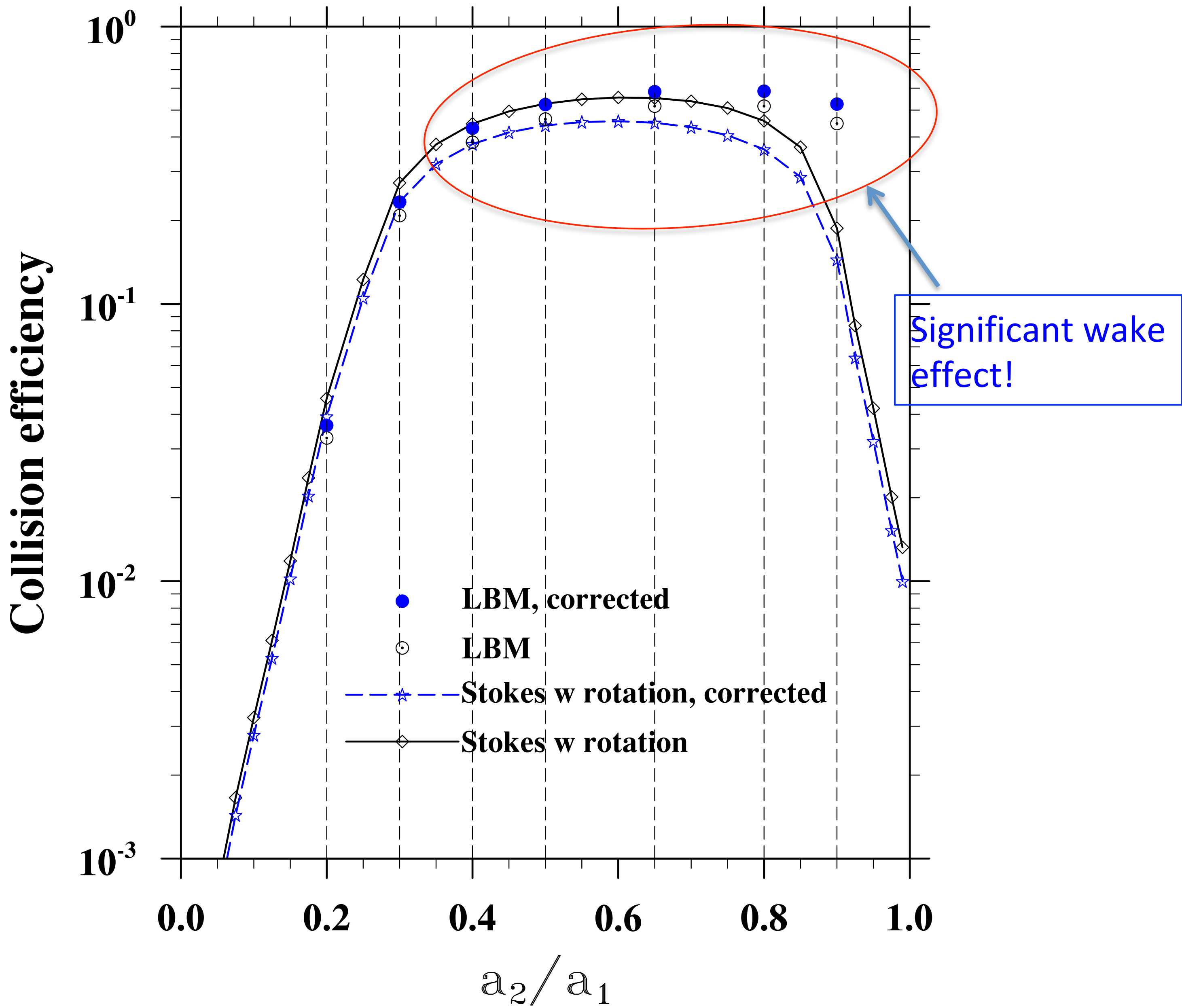
$\frac{a_2}{a_1}$	LBM	Exact Stokes	LBM corrected $\text{LBM}\times\left[\frac{(W_1-W_2)_{real}}{(W_1-W_2)_{simulated}}\right]^{1.85}$	Stokes corrected $\text{ES}\times\left[\frac{(W_1-W_2)_{real}}{(W_1-W_2)_{Stokes}}\right]^{1.85}$	rel. diff
0.20	0.03285	0.04566	0.03647	0.03929	−7.2%
0.30	0.2082	0.2731	0.2330	0.2336	−0.3%
0.40	0.3829	0.4463	0.4301	0.3771	+14.1%
0.50	0.4641	0.5273	0.5235	0.4456	+17.5%
0.65	0.5166	0.5526	0.5827	0.4500	+29.5%
0.80	0.5166	0.4572	0.5850	0.3609	+62.1%
0.90	0.4641	0.1875	0.5255	0.1446	+263.4%

Comparison of corrected collision efficiency

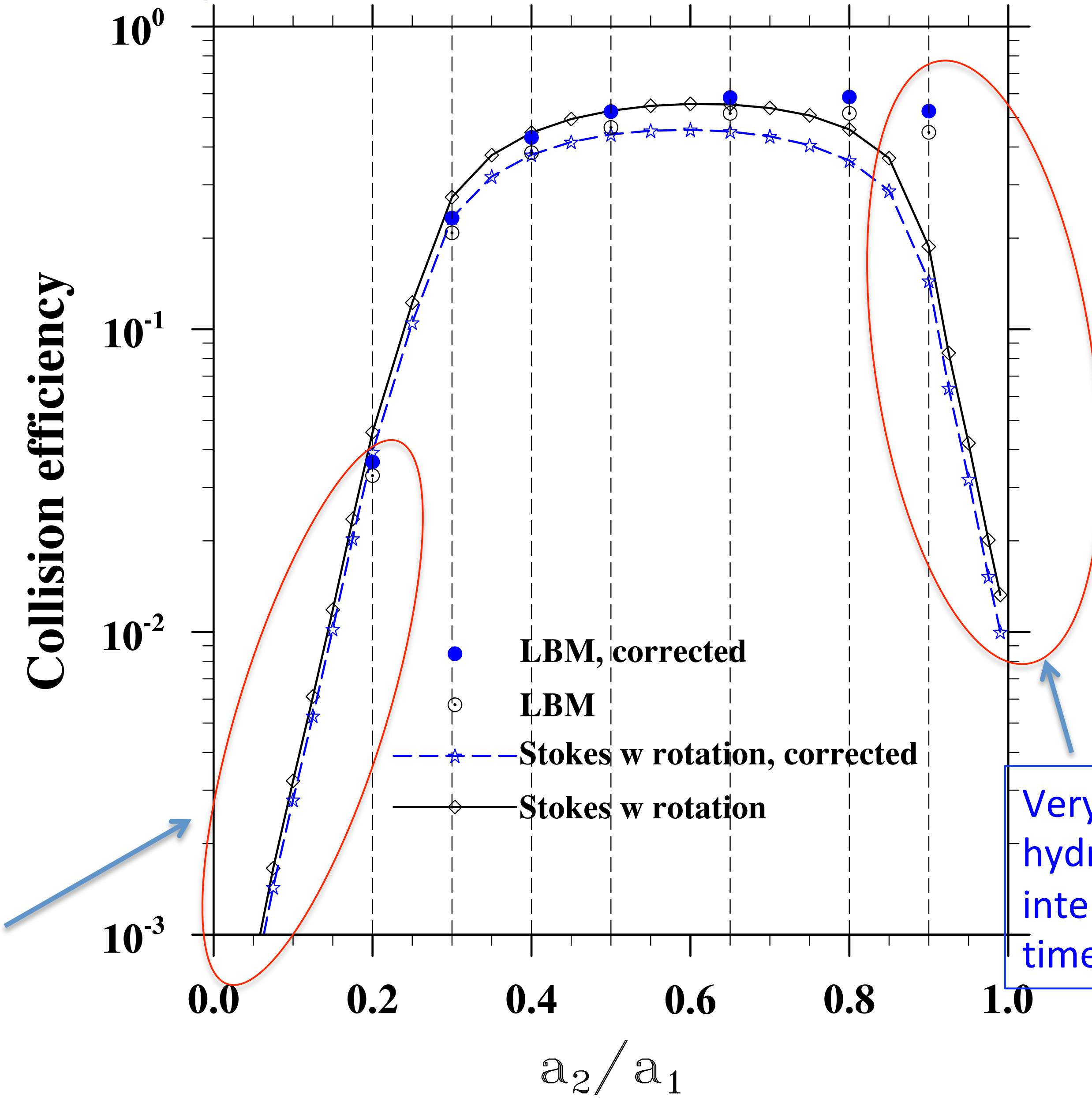


For small ratios, corrected LBM data agree well with the corrected Stokes flow results.

Comparison of corrected collision efficiency



Computational challenges



Resolving both large and small droplets and yet covering a large domain.

Very long hydrodynamic interaction time.

Enhancement factors

$$a_1 = 30\ \mu m$$

$\frac{a_2}{a_1}$	LBM corrected	Stokes corrected	$\frac{\text{LBM corrected}}{\text{Stokes corrected}}$	$\eta^{Turb}(ISM)$
0.20	0.03647	0.03929	0.93	1.245 / 1.475
0.30	0.2330	0.2336	1.00	1.148 / 1.187
0.40	0.4301	0.3771	1.14	1.066 / 1.088
0.50	0.5235	0.4456	1.19	1.000 / 1.130
0.65	0.5827	0.4500	1.29	1.042 / 1.273
0.80	0.5850	0.3609	1.62	1.117 / 1.345
0.90	0.5255	0.1446	3.62	1.244 / 1.501

For nearly equal sizes, the wake effect can be much stronger than the enhancement due to turbulence based on ISM (accounting both geometric collision and collision efficiency).

Summary (1)

An interface-resolved direct numerical simulation approach is applied to simulate coalescence of cloud droplets

- Lattice Boltzmann method with interpolated bounce-back
- Near-field lubrication force (not resolved) is corrected and validated
- Domain shifting
- Domain stretching during initialization: the droplets to reach to steady-state terminal velocity before hydrodynamic interaction
- Accelerate the initialization process by artificially augmenting ***g***

→ Make the best use of finite simulation domain, and initialization more efficient

Still further investigation is needed to check sensitivity of results to

Grid resolution
Domain size
Details of lubrication correction model

Summary (2)

Collision efficiencies for droplets pairs of a_1=30 μm and several a_2/a_1 have been obtained

- Initial vertical distance $20(a_1+a_2)$, coalescence gap = $0.001a_1$
- Two deviations from Stokes disturbance flows must be considered
  - Terminal velocity reduction [14% to 23%]
  - Wake effect [for $a_2/a_1 > 0.50$, may increase efficiency by a factor of 3!]
- A correction to previous Stokes flow results is suggested
- A correction to IR-DNS data is also suggested to remove the effect of finite simulation domain size

→ **After these corrections:**
Collision efficiencies for small a_2/a_1 ratios are in good agreement
Collision efficiencies for large a_2/a_1 ratios are significantly larger due to the wake effect

Yes, we can simulate the collision efficiency of cloud droplets

Some take-home messages

The problem of turbulent collision efficiency remains largely unsolved

A multiscale problem, computationally challenging
How to incorporate disturbance flows accurately and efficiently?

Better methods are being developed, actual computations remain to be done.

How does turbulence enhance the collision-coalescence rate of cloud droplets?

Enhancing geometric collision (relative motion, local clustering)
Enhancing collision efficiency

Coupling turbulence effects and hydrodynamic interactions (i.e., wakes)
Droplet clustering → local strong long- and short-range interactions → large efficiency

→ A narrow droplet size spectrum may not be a bottleneck for collision-coalescence in a turbulent flow!