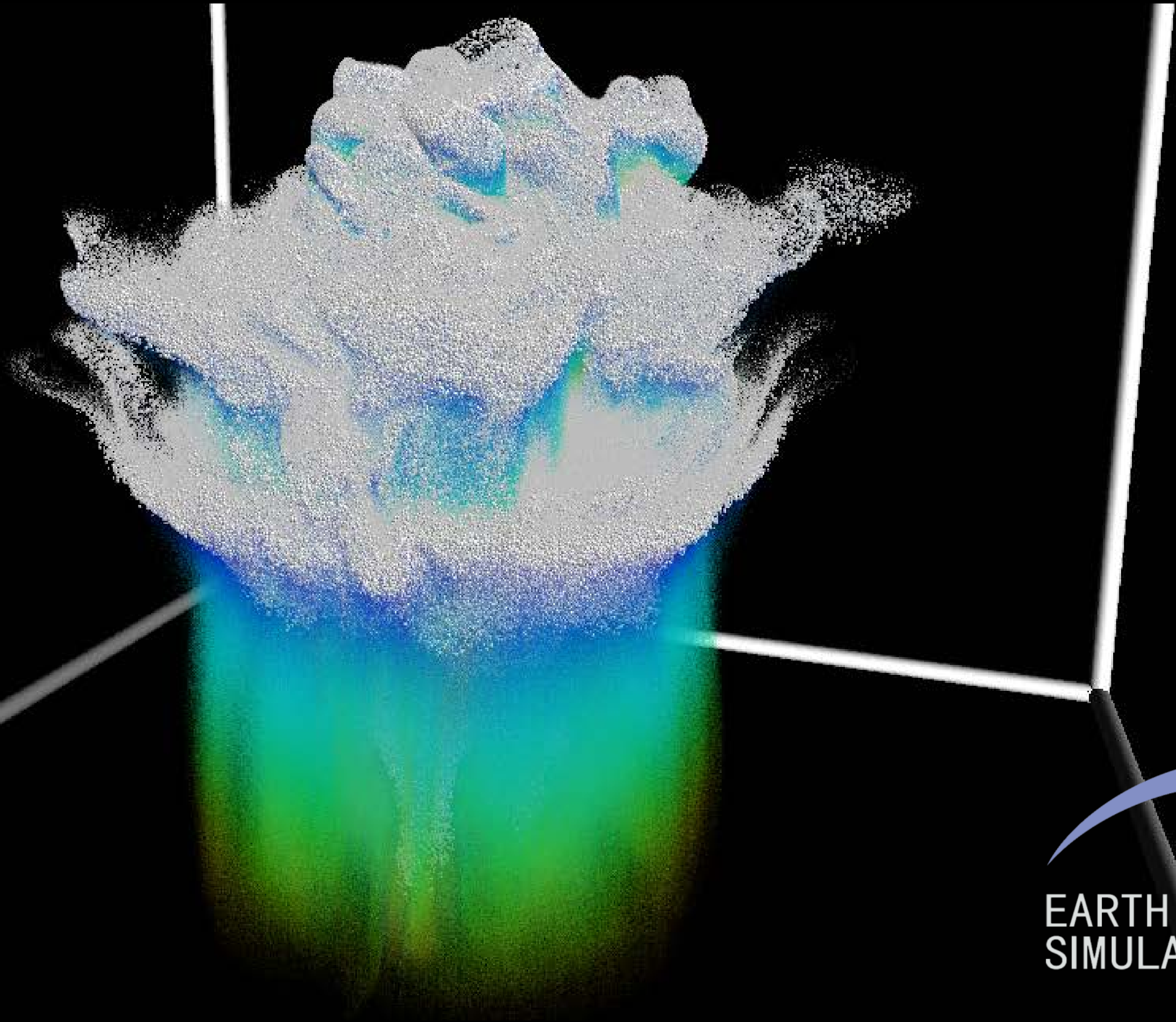
Particle-based and probabilistic methods for warm-rain cloud microphysics

Shin-ichiro Shima,
U. of Hyogo / RIKEN / Osaka U.



EARTH SIMULATOR

Abstract

- Particle-based and probabilistic approach to simulate cloud-microphysics is introduced
- Special focus on the Super-Droplet Method (SDM) (S.S. et al., 2009; S.S. 2008)
- Computational cost of SDM is discussed.

Outline

1. Physics of Clouds Overview
2. Basic Equations of Clouds
3. Super-Droplet Method
4. Other Methods
5. Computational Cost of SDM
6. Concluding Remarks

1. Physics of Clouds Overview

Cloud Dynamics

dry air, vapor, trace gas.

interaction

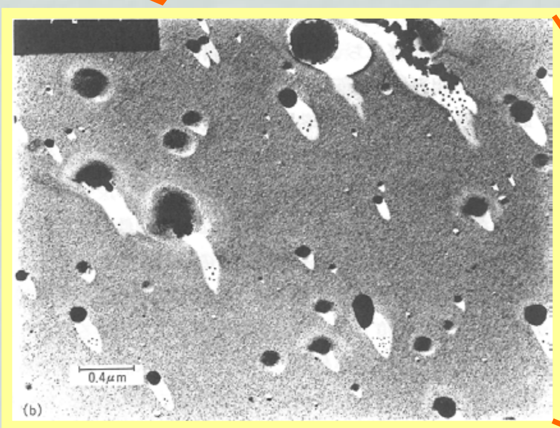
Cloud Microphysics

particles (aerosol/cloud/precipitation)

nucleation from gases
or rolling up of dusts

chemical
reactions

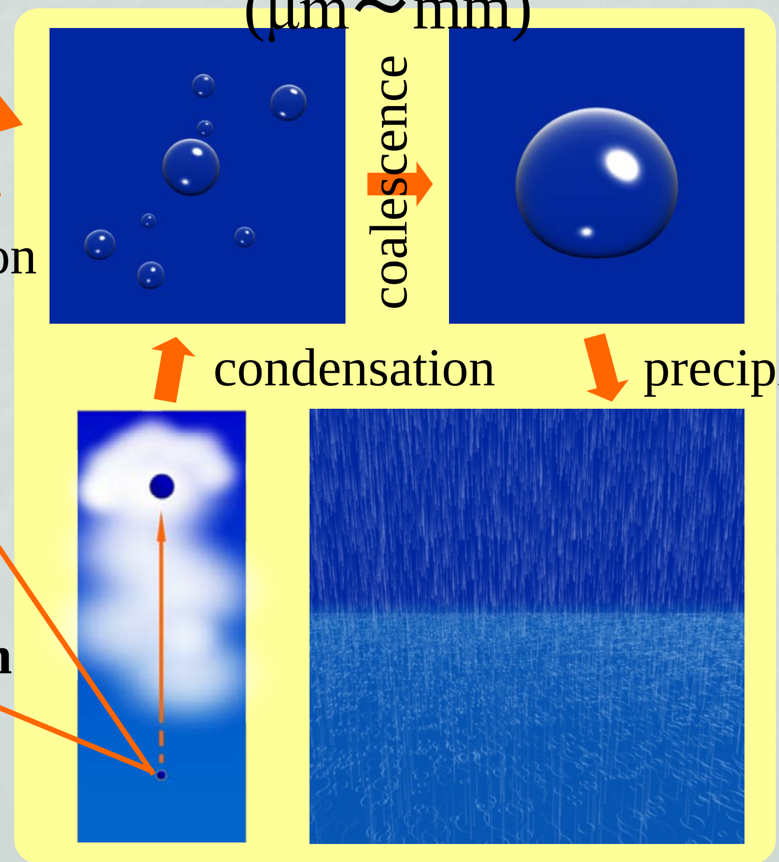
evaporation



**aerosol-
cloud
interaction**

aerosols (nm～μm)
(S.Twomey,1977:Atmospheric Aerosols, Elsevier Pub. Co)

(μm～mm)



2. Basic Equations of Clouds

2.1. Mesoscopic Description of Cloud Microphysics

Basic equations are written down in a general form

State variables

Particles (or Droplets): Generic name for Aerosols/Cloud/Precipitation particles

$\boldsymbol{x}(t)$: the position of the particle

$\boldsymbol{a}(t)=\{a^{(1)}(t), a^{(2)}(t), \ldots, a^{(d)}(t)\}$: the state of the particle, that is specified by d number of attributes

$N_r(t)$: total number of particles at a time t

Then, **the state of the cloud microphysical system is determined by**

$$\{(\boldsymbol{x}_i(t), \boldsymbol{a}_i(t)) | i = 1, 2, \ldots, N_r(t)\}$$

Individual dynamics of particles

Time evolution without particle-particle interaction

It is affected by the ambient atmosphere.

These can be expressed by the following form:

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i, \qquad \frac{d\boldsymbol{a}_i}{dt} = \boldsymbol{f}(\boldsymbol{a}_i), \qquad i = 1, 2, \ldots, N_r(t).$$

Here, $\boldsymbol{v}_i$ is the velocity of the particle.

$\boldsymbol{v}_i$ is regarded as one of the attribute variables

In general, $\boldsymbol{f}$ is an atmosphere (fluid field) dependent function.

Coalescence of particles

The only interaction between particles

Assuming that the particles are well mixed by the atmospheric turbulence, coalescence can be regarded as a stochastic event

$$\begin{aligned} P_{jk} =& C(\boldsymbol{a}_j, \boldsymbol{a}_k)|\mathbf{v}_j - \mathbf{v}_k|\frac{\Delta t}{\Delta V} \\ =& K(\boldsymbol{a}_j, \boldsymbol{a}_k)\frac{\Delta t}{\Delta V} \\ =& \text{probability that droplet } j \text{ and } k \\ & \text{inside a small region } \Delta V \text{ will coalesce} \\ & \text{in a short time interval } (t, t+\Delta t). \end{aligned}$$

All the pair (*j*,*k*) inside Δ*V* have some possibility to coalesce

In general C and K also depend on fluid field

These are the mesoscopic basic equations of cloud microphysics

Below is another equivalent representation of the governing law

Stochastic Coalescence Equation (SCE, Smoluchowski eq.)

Let $n(\boldsymbol{a},\boldsymbol{x},t)$ be the number density of particles at time t, at $\boldsymbol{x}$, with attribute $\boldsymbol{a}$, then below can be derived:

$$\frac{\partial n(\boldsymbol{a},\boldsymbol{x},t)}{\partial t} + \nabla_x \cdot \{\boldsymbol{v}n\} + \nabla_a \cdot \{\boldsymbol{f}n\} = \frac{1}{2}\int d^d a' n(\boldsymbol{a}')n(\boldsymbol{a}'')K(\boldsymbol{a}',\boldsymbol{a}'') - n(\boldsymbol{a})\int d^d a' n(\boldsymbol{a}')K(\boldsymbol{a},\boldsymbol{a}').$$

Here, $\boldsymbol{a}'+\boldsymbol{a}''=\boldsymbol{a}$ ("+" denotes coalescence). Also, decoupling assumption $p(n_1,\boldsymbol{a}_1,n_2,\boldsymbol{a}_2)=p(n_1,\boldsymbol{a}_1)p(n_2,\boldsymbol{a}_2)$ etc. is adopted.

2.2. Minimal Warm Cloud Microphysics

As a concrete example, the most fundamental warm cloud microphysical processes are introduced.

State variables

$$\{(\boldsymbol{x}_i(t), \boldsymbol{a}_i(t)) | i = 1, 2, \ldots, N_r(t)\}$$

$\boldsymbol{x}(t)$: the position of the particle

State of a particle is described by 5 attribute variables: $\boldsymbol{a}(t)$={velocity v, equivalent radius of water R, mass of ammonium sulfate M}

Typical size range

Aerosols: 1nm to 1μm

Cloud droplets: 1μm to 50μm

Rain droplets: 50μm to 1mm

Individual dynamics of particles

a). Advection by the wind and gravity

Adopt the terminal velocity approximation

→ Number of independent attributes reduces to 2

Important for precipitation (rain droplets falling)

b). Condensation/evaporation of vapor

Depending on the saturation ratio, particles absorb/evolve vapor from the ambient atmosphere

Important for converting aerosols to cloud drops

Coalescence of particles

c). Coalescence by the gravitational settling

Dominant for converting cloud droplets to rain droplets

a) Motion of particles by the wind and gravity

Let F_D be the air resistance. The motion eq. of a particle is

$$m_i d\boldsymbol{v}_i/dt = m_i\boldsymbol{g} + F_D, \quad d\boldsymbol{x}_i/dt = \boldsymbol{v}_i.$$

If particles are always moving with the terminal velocity,

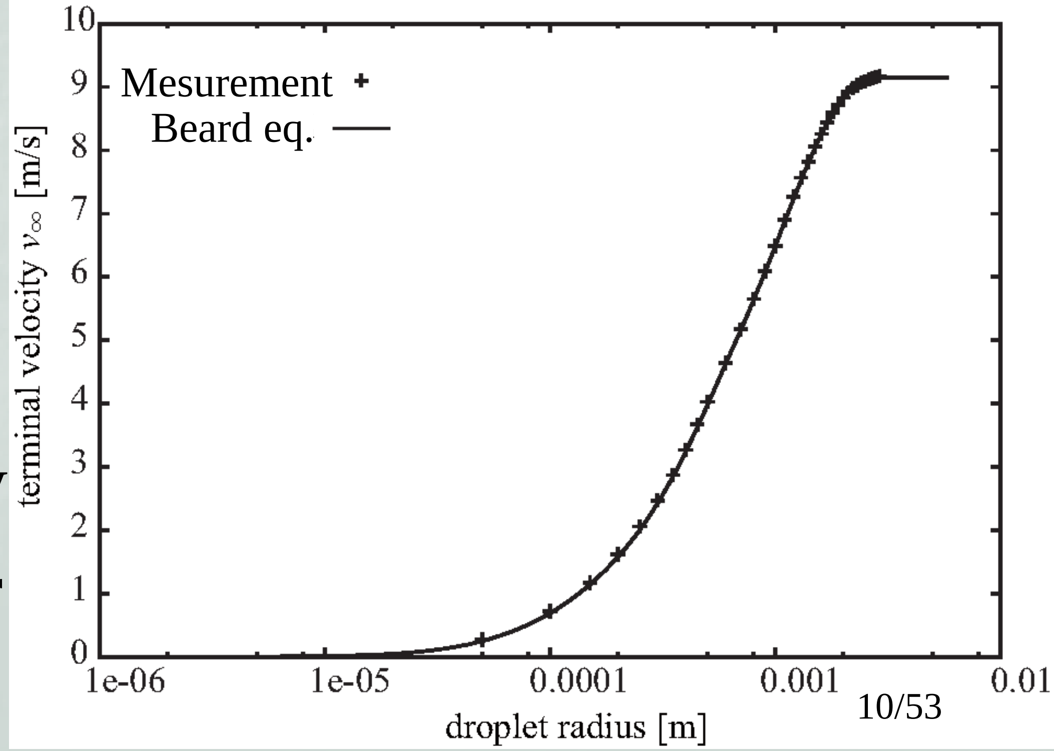
$$\boldsymbol{v}_i(t) = \boldsymbol{U}_i^* - \hat{\boldsymbol{z}} v_\infty(R_i, T_i^*, P_i^*), \quad d\boldsymbol{x}_i/dt = \boldsymbol{v}_i,$$

$\boldsymbol{U}_i^*$, T_i^*, P_i^* are the wind velocity, temperature, pressure

$v_\infty(R_i,T_i^*,P_i^*)$ is the terminal velocity.

Beard's formula (1976) is famous

Terminal velocity suddenly increases when it's larger than 100μm → rain



b) Condensation and evaporation of water from droplets

When oversaturated, vapor condensates to droplets. When undersaturated, vapor evaporates from droplets.

Here, the effective saturation vapor pressure is affected by the curvature effect and dissolution effect of aerosols

Based on Köhler's theory(1936), we can derive

$$R_i \frac{dR_i}{dt} = \frac{1}{F_k(T_i^*) + F_d(T_i^*)} \left\{ S_i^* - \frac{e_s'(R_i, M_i, T_i^*)}{e_s(T_i^*)} \right\},$$

$$\frac{e_s'(R_i, M_i, T_i^*)}{e_s(T_i^*)} = 1 + \frac{a(T_i^*)}{R_i} - \frac{b(M_i)}{R_i^3},$$

$$F_k(T_i^*) = \left(\frac{L}{R_v T_i^*} - 1 \right) \frac{L \rho_{\mathrm{liq}}}{K T_i^*}, \quad F_d(T_i^*) = \frac{\rho_{\mathrm{liq}} R_v T_i^*}{D e_s(T_i^*)}.$$

…cont. (Condensation and evaporation of water…)

S_i^*: saturation ratio at the position of the particle i

e_s'/e_s: ratio of effective saturation ratio and saturation ratio of the bulk

$a(T_i^*)/R_i$: expressing the increase of effective saturation ratio caused by the curvature effect of the droplet

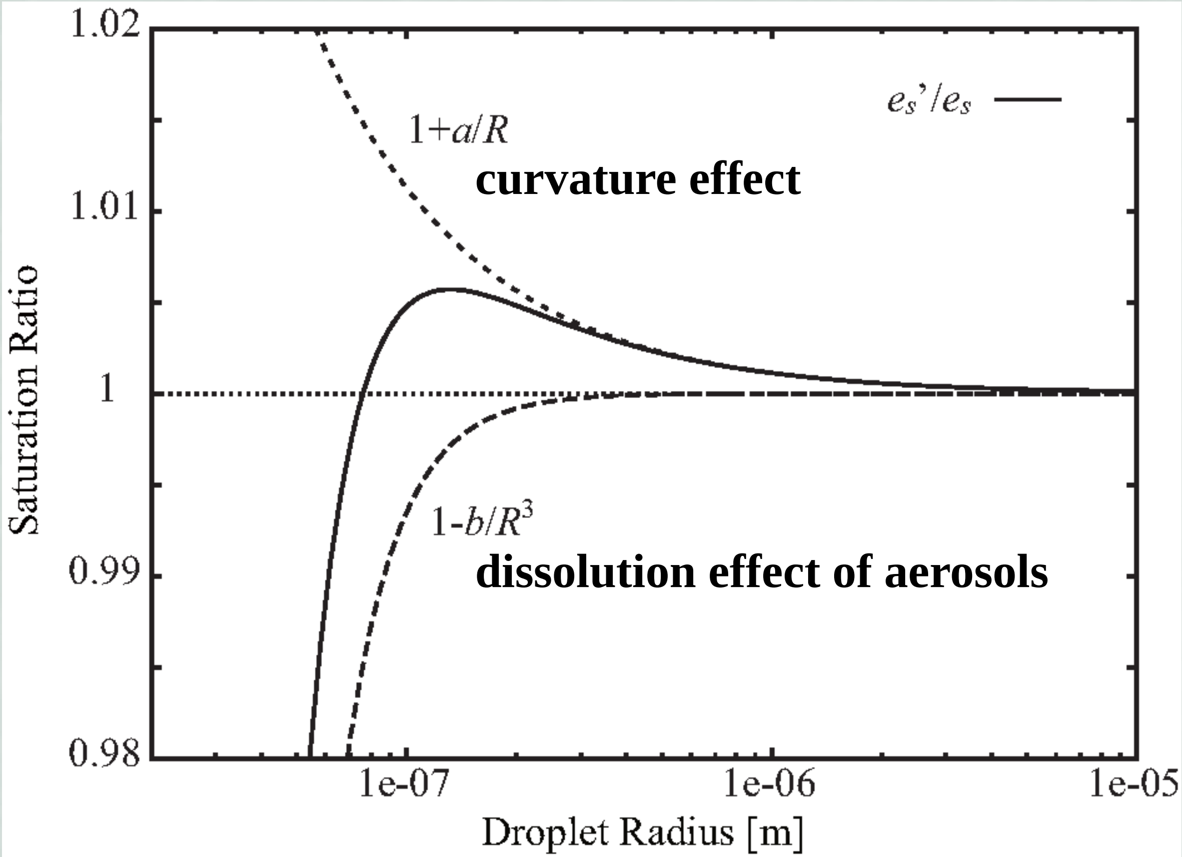
$b(M_i)/R_i^3$: expressing the decrease of effective saturation ratio caused by the dissolution effect of ammonium sulfate

F_k: coefficient relating to the thermal conduction

F_d: coefficient relating to the vapor diffusion

…cont. (Condensation and evaporation of water…)

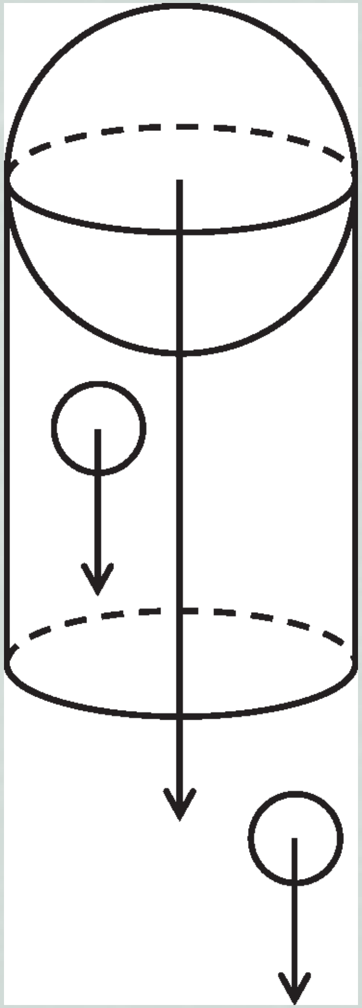
Köhler curve for a droplet containing ammonium sulfate 10^{-16}g at 293K is



Tiny droplet is stable even if it's unsaturated. Cloud droplets won't be created if oversaturation of some extent occurs

c) Coalescence of particles by the gravitational settling

Bigger particles sweep smaller particles because of the difference of their terminal velocities



Consider two particles j and k in a volume ΔV

2 particles sweep the volume $\pi(R_j+R_k)^2|\boldsymbol{v}_j-\boldsymbol{v}_k|\Delta t$ during a small time interval $(t,t+\Delta t)$

If ΔV is small enough, particles are well mixed by the atmospheric turbulence

Thus, the probability that the coalescence occurs is the ration of sweep volume and ΔV

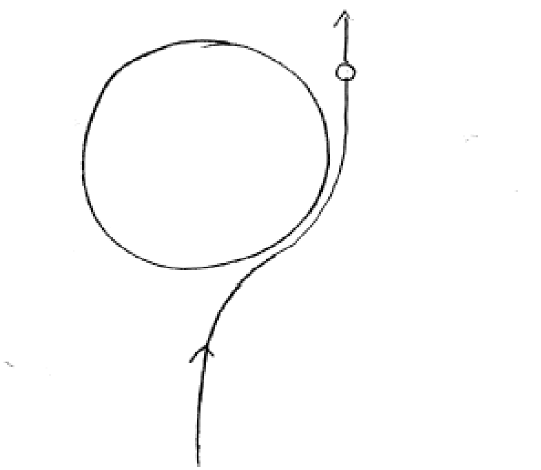
$$P_{jk} = \pi(R_j + R_k)^2 |\boldsymbol{v}_j - \boldsymbol{v}_k| \frac{\Delta t}{\Delta V}.$$

However,

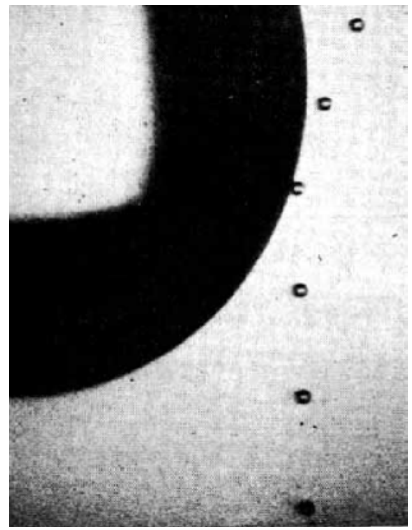
…cont. (Coalescence of particles by the gravitational settling)

this evaluation is not good for small droplets

Small droplet could swept aside, or bounce



swept aside along the flow



bounce on the surface

collision and bounce of small droplet (35μm in radius) and large droplet (1.75mm in radius). (adapted from Whelpdale and List, 1971)

Incorporate this by the coalescence efficiency $E(R_j, R_k)$

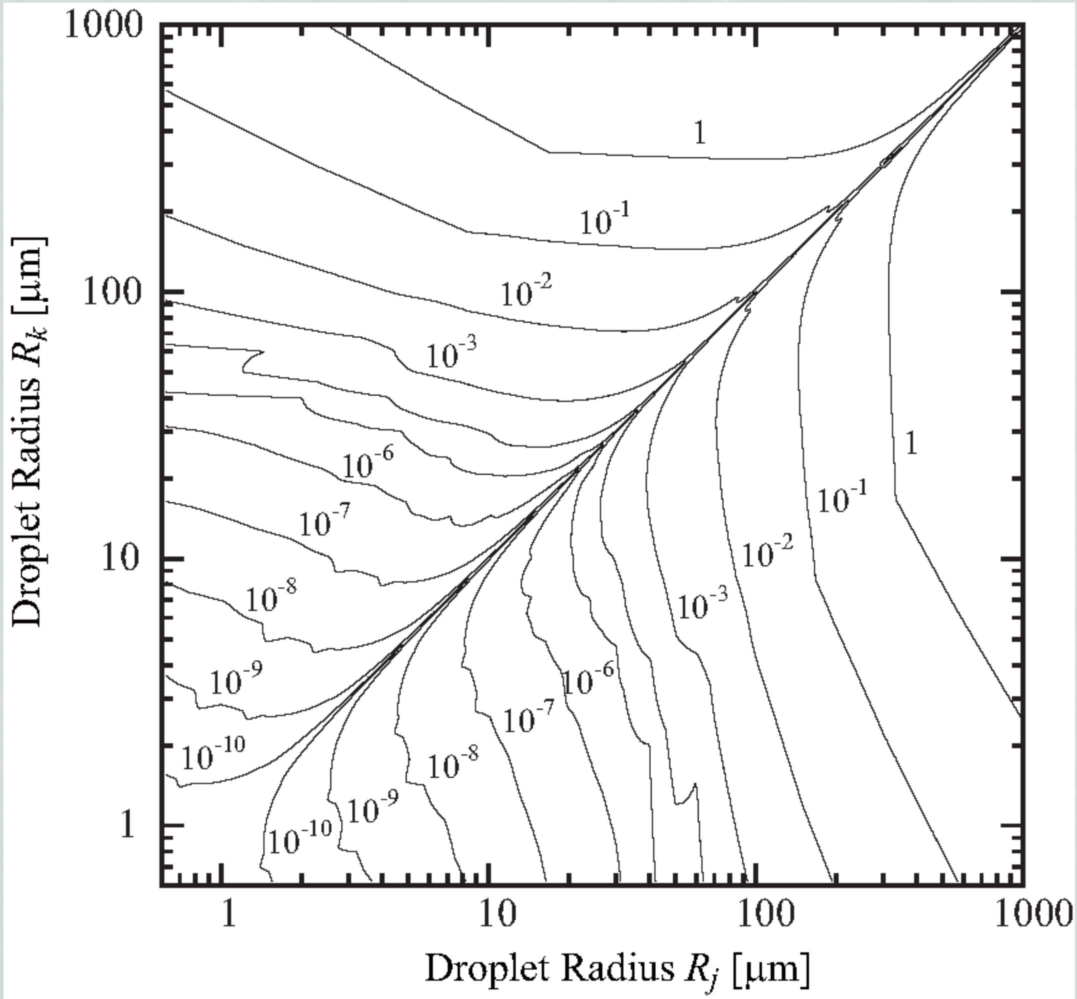
$$P_{jk} = E(R_j, R_k)\pi(R_j + R_k)^2|\boldsymbol{v}_j - \boldsymbol{v}_k|\frac{\Delta t}{\Delta V}.$$

e.g., theories of Davis(1972), Jonas(1972), Hall(1980)

…cont. (Coalescence of particles by the gravitational settling)

Contour plot of P_{jk} as a function of R_j and R_k

ΔV=1cm^3, Δt=1s, 101.3kPa, 20℃.



- Same size droplets won't coalesce
- Small droplets seldom coalesce
  - Droplets larger than 10μm are necessary for rain
- Clustering of inertia particles by turbulence could be important (e.g., Falkovich et al., 2002)

2.3. Basic Equations of the Cloud Dynamics

Compressible Navier-Stokes equation for moist air

$$\rho \frac{D\vec{\mathbf{v}}}{Dt} = -\nabla P - \rho \vec{\mathbf{g}} + \underline{S_m},$$ motion eq.

momentum coupling

$$P = \rho R_d T,$$ eq. of state

$$\frac{D\theta}{Dt} = \underline{-\frac{L}{c_p \Pi} S_v},$$ energy eq.

thermal coupling

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \vec{\mathbf{v}},$$ continuity eq.

$$\frac{Dq_v}{Dt} = \underline{S_v}.$$ mass coupling

$\boxed{S_m(\boldsymbol{r},t),\ S_v(\boldsymbol{r},t)}$ coupling term to microphysics process

- $\rho = \rho_d + \rho_v$: densitiy of moist air
- $q_v = \rho_v / \rho$: mixing ratio of vapor
- $\vec{\mathbf{v}}$: wind velocity
- T : temperature
- θ : potential temperature
- $\Pi = (p / p_0)^{R_d / c_p}$ Exner function
- ρ_w : density of liquid water
- S_v : source term for vapor from liquid
- $\vec{\mathbf{g}}$: gravitational constant
- R_d : gas constant for dry air
- c_p : isobaric specific heat
- L : latent heat of vapor

density of liquid water / unit space volume

mass of evaporated liquid water/ unit space volume /unit time/ρ

3. Super-Droplet Method

SDM is introduced in 2 steps:

concept of super-droplets and its numerical implementation

3.1. Governing Law of the Super-Droplet World

Basic idea

Coarse-grain unnecessary degrees of freedom

Super-droplet

SD has **multiplicity ξ**, position $\boldsymbol{x}$, and attribute $\boldsymbol{a}$

Each SD represents ξ number of real-droplets $(\boldsymbol{x},\boldsymbol{a})$

Population of real-droplets $\{(\boldsymbol{x}_i(t), \boldsymbol{a}_i(t))|i=1,2,\ldots,N_r(t)\}$ is represented by the SD population. ($N_s(t)$ is the num of SDs)

$$\{(\xi_i(t), \boldsymbol{x}_i(t), \boldsymbol{a}_i(t))|i = 1, 2, \ldots, N_s(t)\}$$

SD can be regarded as a weighted sample of RDs

Note that ξ is time dependent (Detail follows)

Dynamics of super-droplets

Individual dynamics

Same as real-droplets, they obey

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i, \qquad \frac{d\boldsymbol{a}_i}{dt} = \boldsymbol{f}(\boldsymbol{a}_i), \quad i = 1, 2, \ldots, N_s(t).$$

Coalescence

SDs also undergo stochastic coalesce (detail follows)

$$\begin{aligned} P^{(s)}_{jk} = &\text{probability that super-droplets } j \text{ and } k \\ &\text{inside a small region } \Delta V \text{ will coalesce} \\ &\text{in a short time interval } (t, t+\Delta t). \end{aligned}$$

The way they coalesce is different

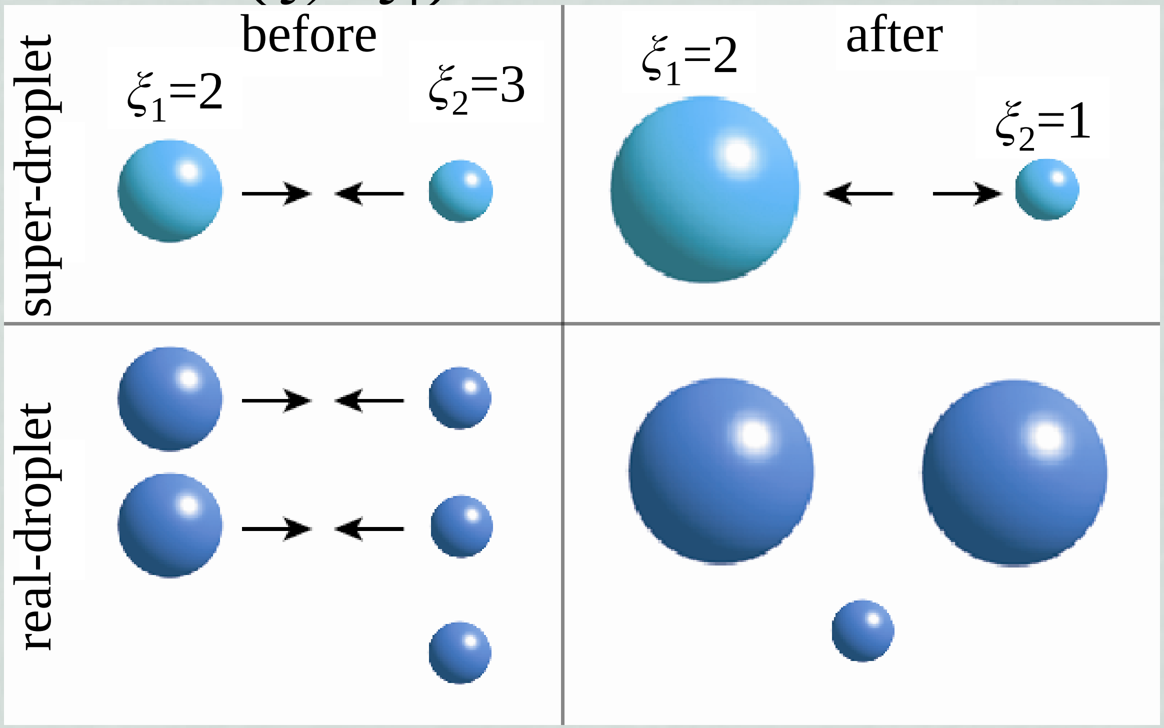
The probability is different

But, **the expected results is the same**

Definition of how a pair of SDs coalesce

Let ξ_1 and $\xi_2(>\xi_1)$ be the multiplicity of the two SDs

After the coalescence event, we define that a big SD with ξ_1, and a SD with $(\xi_2-\xi_1)$ with no size difference are created



SD num is almost conserved though RD num decreases

When $\xi_2=\xi_1$, we split the remaining SD

We now adjust the probability to get a consistent results

Definition of the coalescence probability of super-droplets

Requiring that the expected num of coalesced RDs becomes the same, we get

$$\boxed{P^{(s)}_{jk} := \max(\xi_j, \xi_k) P_{jk}}$$

Check) Consider coalescence between ξ_j num of RD $\boldsymbol{a}_j$ and ξ_k num of RD $\boldsymbol{a}_k$. Expected num of coalesced pairs is

$$E_{jk} = \xi_j \xi_k P_{jk} \quad \leftarrow \textbf{Real World}$$

Coalescence of SDs (ξ_j, $\boldsymbol{a}_j$) and (ξ_k, $\boldsymbol{a}_k$) corresponds to coalescence of min(ξ_j, ξ_k) pairs of RD $\boldsymbol{a}_j$ and $\boldsymbol{a}_k$

Thus, the expected num of coalesced RD num in the super-droplet world becomes

$$\begin{aligned} E^{(s)}_{jk} &= \min(\xi_j, \xi_k) P^{(s)}_{jk} \quad \leftarrow \textbf{Super-Droplet World} \\ &= \min(\xi_j, \xi_k) \max(\xi_j, \xi_k) P_{jk} \\ &= \xi_j \xi_k P_{jk} \\ &= E_{jk} \end{aligned}$$

3.2. Numerical Implementation of the SDM

Outlook

- Cloud microphysics (= Super-Droplet Method)
  - Individual dynamics

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i, \quad \frac{d\boldsymbol{a}_i}{dt} = \boldsymbol{f}(\boldsymbol{a}_i), \quad i = 1, 2, \ldots, N_s(t).$$

    - Solve these ODEs for each SD
  - Coalescence
    - **A novel Monte Carlo scheme is developed to solve this stochastic process of SDs** (Detail later)

- Cloud Dynamics
  - Solve the Navier-Stokes eq. for atmospheric fluid
  - When simulating a whole cloud, we need to resort to some sub-grid scale turbulence model.

Operator Splitting

- Evaluate each process individually, based on Trotter's factorization formula
- Let $X(t)$ be the state of our system (Everything included)
- Let Δt be the least common multiple time step and repeat

$$X^{(1)}(t+\Delta t) = A(\Delta t)X(t), \quad \text{(update fluid)}$$

$$X^{(2)}(t+\Delta t) = B(\Delta t)X^{(1)}(t+\Delta t), \quad \text{(coalescence)}$$

$$X^{(3)}(t+\Delta t) = C(\Delta t)X^{(2)}(t+\Delta t), \quad \text{(condensation / evaporation)}$$

$$X(t+\Delta t) = D(\Delta t)X^{(3)}(t+\Delta t), \quad \text{(advection / sedimentation)}$$

  - Here, A,B,C,D denote their time propagation operators
- The global error is $O(\Delta t)$
  - Employing higher order formula, accuracy can be improved

Cloud Dynamics

Basic equations

$$\rho \frac{D\mathbf{U}}{Dt} = -\nabla P - (\rho + \rho_w)\mathbf{g} + \lambda \nabla^2 \mathbf{U},$$

$$P = \rho R_d T,$$

$$\frac{D\theta}{Dt} = -\frac{L}{c_p \Pi} S_v + \kappa \nabla^2 \theta,$$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{U},$$

$$\frac{Dq_v}{Dt} = S_v + \kappa \nabla^2 q_v.$$

Numerical scheme

- Evaluate all the terms except pink terms with Δt_f
- Green term is calculated from the super-droplets
- e.g., Space: 2nd order center difference+LES, Time: 4th order Runge-Kutta

Advection and Sedimentation in Terminal Velocity

Basic eq.

$$m_i \frac{d\mathbf{v}_i}{dt} = m_i \mathbf{g} + \mathbf{F}_D(\mathbf{v}_i, \mathbf{U}(\mathbf{x}_i), R_i), \qquad \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i,$$

Numerical scheme

$$\mathbf{v}_i(t) = \mathbf{U}_i^* - \hat{\mathbf{z}} v_\infty(R_i(t))$$

$$\mathbf{x}_i(t + \Delta t_m) = \mathbf{x}_i(t) + \Delta t_m \mathbf{v}_i(t)$$

Condensation/Evaporation

Basic eqs.

$$R_i \frac{dR_i}{dt} = \frac{(S-1) - \frac{a}{R_i} + \frac{b}{R_i^3}}{F_k + F_d},$$

$$F_k = \left(\frac{L}{R_v T} - 1\right)\frac{L\rho_{\mathrm{liq}}}{KT}, \quad F_d = \frac{\rho_{\mathrm{liq}} R_v T}{D e_s(T)}.$$

$$\frac{D\theta}{Dt} = -\frac{L}{c_p \Pi} S_v + \kappa \nabla^2 \theta,$$

$$S_v(\mathbf{x}, t) := \frac{-1}{\rho(\mathbf{x}, t)} \sum_{i=1}^{N_r} \frac{dm_i(t)}{dt} \delta^3(\mathbf{x} - \mathbf{x}_i(t)).$$

$$\frac{Dq_v}{Dt} = S_v + \kappa \nabla^2 q_v.$$

Numerical scheme (Implicitly for SDs, explicitly for fluids)

$$\frac{R_i^2(t+\Delta t_g) - R_i^2(t)}{2\Delta t_g} = \frac{(S_i^* - 1) - \frac{a(T_i^*)}{R_i(t+\Delta t_g)} + \frac{b(M_i(t))}{R_i^3(t+\Delta t_g)}}{F_k(T_i^*) + F_d(T_i^*)},$$

$$S_v(\mathbf{x}_{lmn}, t) = \frac{-1}{\rho(\mathbf{x}_{lmn}, t)} \sum_{i=1}^{N_s} \xi_i \frac{m_i(t+\Delta t_g) - m_i(t)}{\Delta t_g} w(\mathbf{x}_{lmn} - \mathbf{x}_i(t)).$$

(also update fluid)

$$\theta(\mathbf{x}_{lmn}, t+\Delta t_g) = \theta(\mathbf{x}_{lmn}, t) - \Delta t_g \frac{L S_v(\mathbf{x}_{lmn}, t)}{c_p \Pi(\mathbf{x}_{lmn}, t)},$$

$$q_v(\mathbf{x}_{lmn}, t+\Delta t_g) = q_v(\mathbf{x}_{lmn}, t) + \Delta t_g S_v(\mathbf{x}_{lmn}, t).$$

Momentum Transfer from Microphysics

Basic eq.

$$\rho \frac{D\mathbf{U}}{Dt} = -\nabla P - (\rho + \rho_w)\mathbf{g} + \lambda \nabla^2 \mathbf{U},$$

$$\rho_w(\mathbf{x}, t) := \sum_{i=1}^{N_r} m_i(t) \delta^3(\mathbf{x} - \mathbf{x}_i(t)),$$

Numerical scheme

$$\rho_w(\mathbf{x}_{lmn}, t) = \sum_{i=1}^{N_s} \xi_i m_i(t) w(\mathbf{x}_{lmn} - \mathbf{x}_i(t)).$$

Stochastic Coalescence

Basic eq.

$$P_{jk} = E(R_j, R_k)\pi(R_j + R_k)^2 |\boldsymbol{v}_j - \boldsymbol{v}_k| \frac{\Delta t}{\Delta V}.$$

All the pair (j,k) in ΔV have some possibility to coalesce

Translation into a dynamics of SDs $P_{jk}^{(s)} := \max(\xi_j, \xi_k) P_{jk}$

Numerical scheme: **DSMC-like Monte Carlo scheme**

1. Make a list of SDs in each cell. ($O(N_s)$ cost) (The space is divided by a grid.)
2. In each cell, create candidate pairs randomly
3. For each candidate pair, draw a random number and judge whether the coalescence occurs or not.
4. Update of SDs from t to $t+\Delta t_c$

2 techniques here (Detail follows)

Tech A) Pair num reduction and correction to the probability

Let N_s' be the num of SDs in this cell.

Instead of checking all the pairs ${}_{Ns'}C_2$ honestly, we reduce the num of candidate pairs to $[N_s'/2]$

Making a random permutation of SD indices and paring from the front, **we create a non-overlapping pairs**(costs $O(N_s')$)

e.g., (1,2,3,4,5,6,7) → (2,4),(3,5),(7,6),1

With this trick the cost reduces from $O(N_s'^2)$ to $O(N_s')$

In compensation, we scale up the probability of each pair

$$\boxed{p_i := P^{(s)}_{j_i k_i} \frac{N_s'(N_s'-1)}{2} \Big/ \left[\frac{N_s'}{2}\right], \quad i = 1, 2, \ldots, \left[\frac{N_s'}{2}\right].}$$

This assures the consistency of expectation value

$$E[N_{coal}] = \sum_{j=1}^{N's} \sum_{k=1}^{N's} \frac{1}{2} \min(\xi_j, \xi_k) P^{(s)}_{jk} = E\left[\sum_{i=1}^{[N's/2]} \min(\xi_{j_i}, \xi_{k_i}) p_i\right].$$

Tech B) Handling of Multiple Coalescence

To be exact, $p_i>1$ is not allowed, but we accept this.

Let *Ran* be a (0,1) uniform random number

$$q = \begin{cases} \lfloor p_i \rfloor + 1 & \text{if } Ran < p_i - \lfloor p_i \rfloor \\ \lfloor p_i \rfloor & \text{if } Ran \geq p_i - \lfloor p_i \rfloor \end{cases}$$

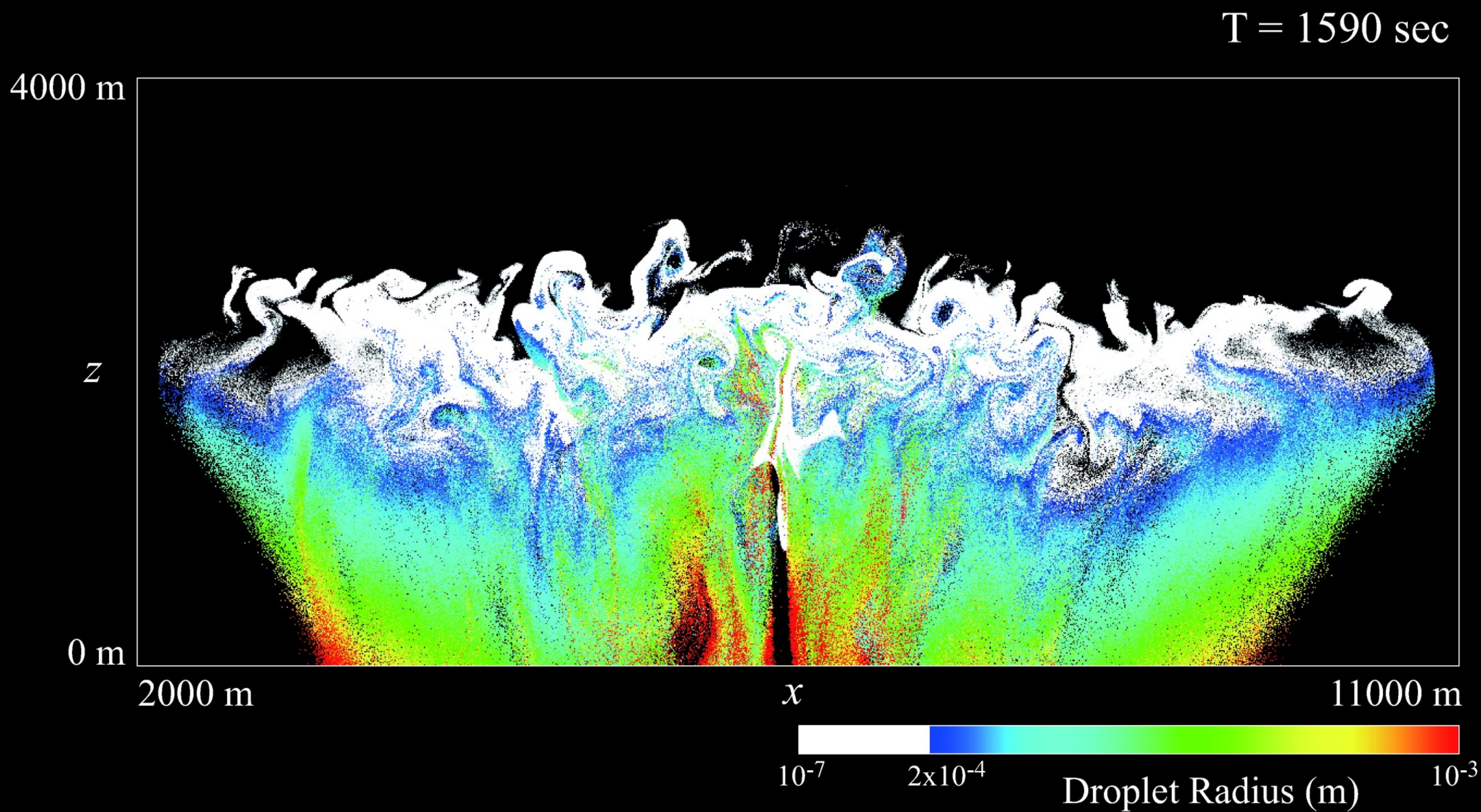
Coalescence occurs q times

e.g. p_i = 2.7, Ran = 0.3, then q=3

This makes our method robust to large Δt_c

Fails when two SD sizes are similar, or when multiplicity is not large enough to accept q times coalescence.

Simulation of a Shallow Maritime Cumulus (2D)



Shallow Maritime Cumulus (3D, Δz= 8 m)

grid: 624x1024x1024, super-droplets: #10^10,

ES 256 nodes (20TFlops in peak)

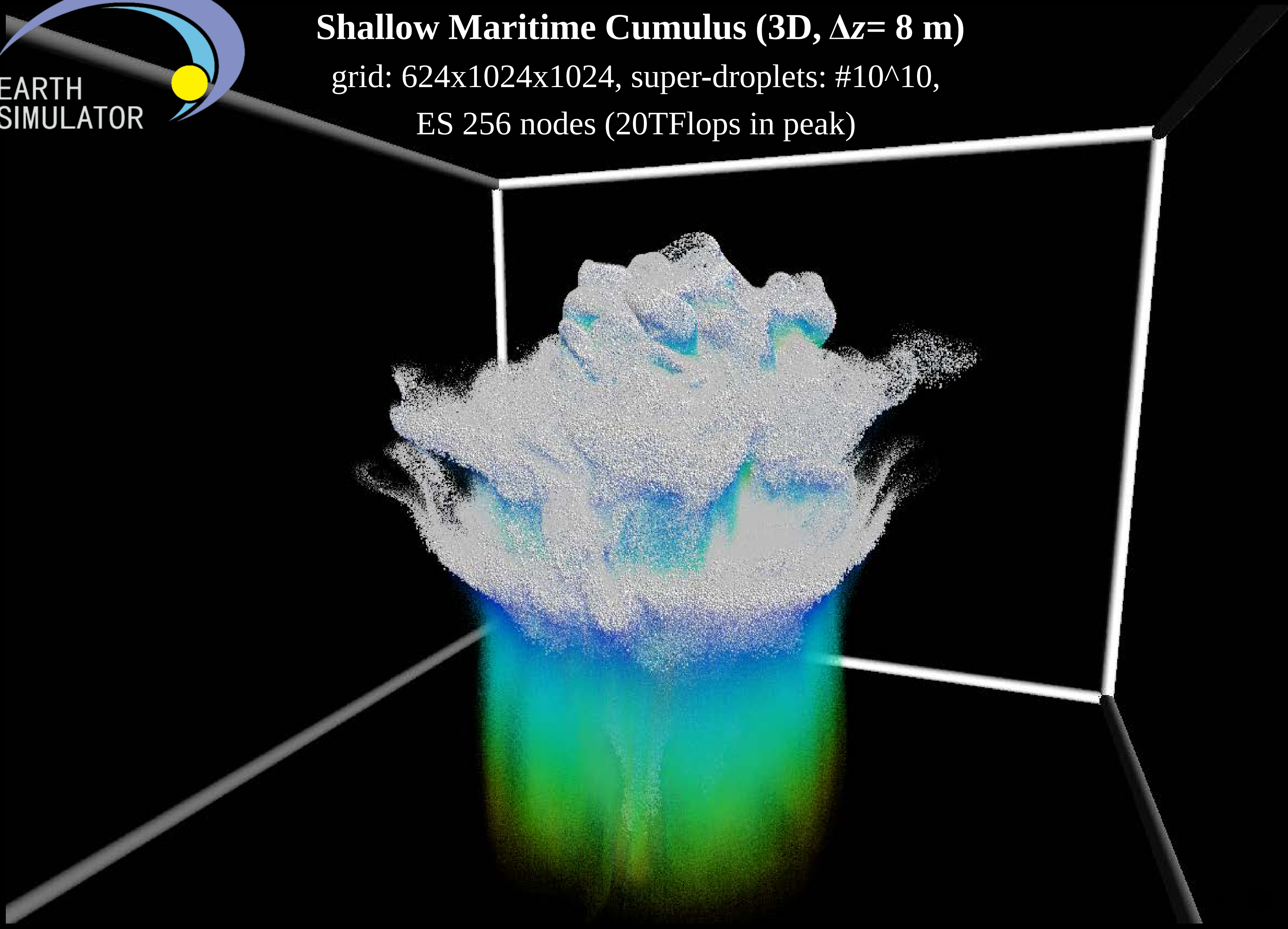
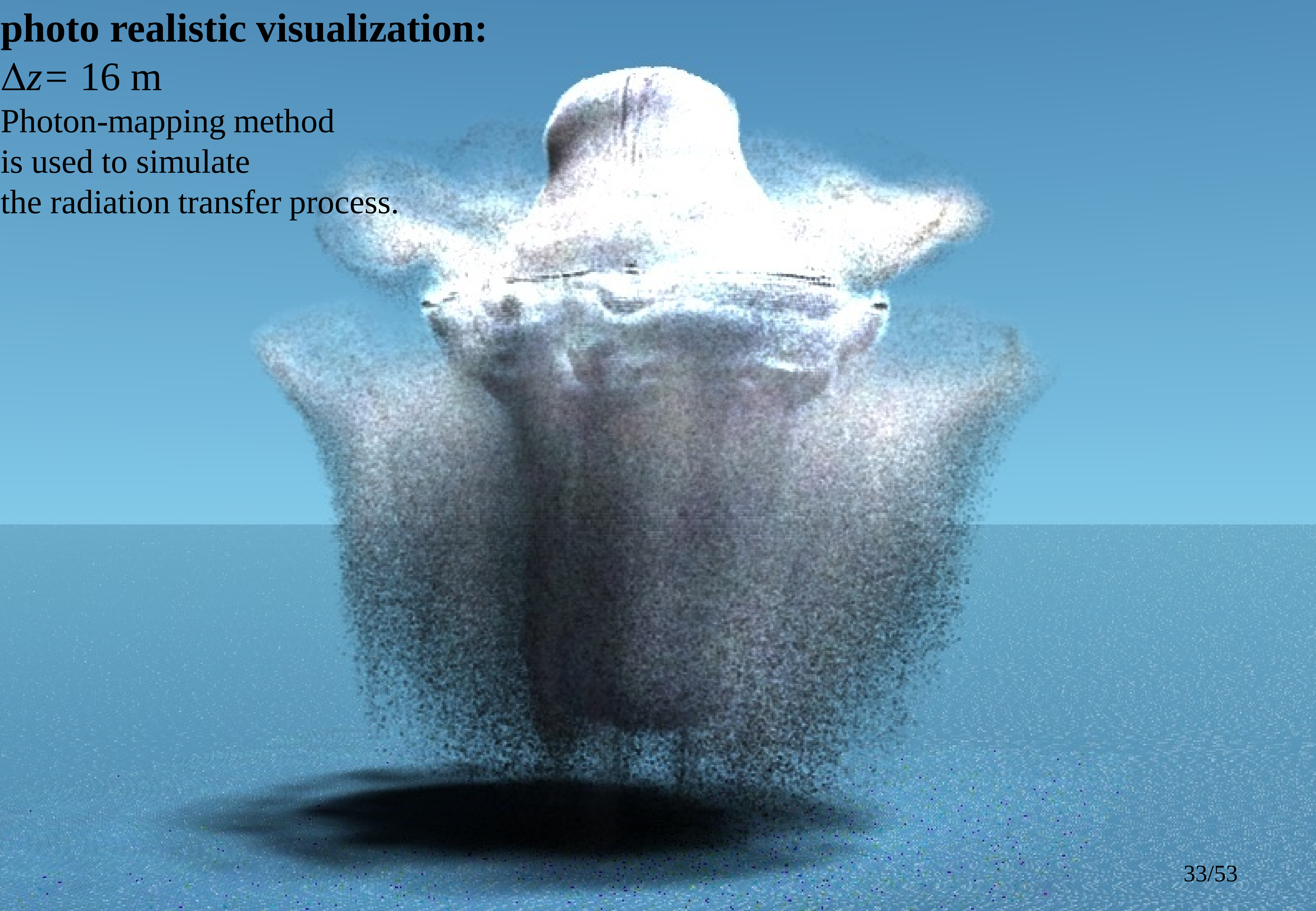


photo realistic visualization:

Δz= 16 m

Photon-mapping method
is used to simulate
the radiation transfer process.



4. Other Methods

(Recap) Stochastic Coalescence Equation

governing equation of the cloud microphysics

$$\frac{\partial n(\boldsymbol{a},\boldsymbol{x},t)}{\partial t} + \nabla_x \cdot \{\boldsymbol{v} n\} + \nabla_a \cdot \{\boldsymbol{f} n\}$$
$$= \frac{1}{2}\int d^{\mathrm{d}}a' n(\boldsymbol{a}')n(\boldsymbol{a}'')K(\boldsymbol{a}',\boldsymbol{a}'')$$
$$- n(\boldsymbol{a})\int d^{\mathrm{d}}a' n(\boldsymbol{a}')K(\boldsymbol{a},\boldsymbol{a}').$$

Here, $n(\boldsymbol{a},\boldsymbol{x},t)$ is the number density; $\boldsymbol{a}=(a_1,a_2,\ldots)$ is the attribute of particles; $\boldsymbol{x}$ is the position in real space; t is time; $\boldsymbol{v}$ is the velocity; $\boldsymbol{f}(\boldsymbol{a})$ is the velocity in attribute space, i.e., $d\boldsymbol{a}/dt=\boldsymbol{f}(\boldsymbol{a})$; $K(\boldsymbol{a},\boldsymbol{a}')$ is the coalescence kernel

SDM is not the only way to solve this equation.

Exact Monte Carlo method (Gillespie1975, Seebelberg1996)

- Calculate the waiting time when the next one pair of coalescence occurs using random numbers
- Most exact
- Enormous cost in computation

Bulk parameterization method (e.g., Kessler 1969)

- Solve a semi-empirical closure equation in lower moments of num density (e.g., number and mass of particles)
- Less accurate
- Very low cost
- **Deriving a reliable bulk model is mathematically challenging but should be pursued**

Spectral (Bin) method (e.g., Bott 1998, 2000)

- Eulerian scheme to solve SCE using a regular grid
- Accurate, but need to cope with numerical diffusion
- Costs a lot if the number of attribute *d* is large (Detail later)
  - **Not suitable to incorporate various cloud microphyics?**

Monte Carlo Spectral (Bin) method (Sato et al., JGR, 2009)

- Monte Carlo scheme is developed to reduce the cost of evaluating the *d*-multiple coalescence integral
  - Pair reduction technique very similar to SDM
  - (Indeed they inspired by SDM)
- Accurate, but need to cope with numerical diffusion
- **Cost is reduced at least to some extent**
  - Maybe another good direction to pursue?

Particle-based Method

- Deterministic: e.g., Andrejczuk et al. 2008, 2010; Riechelmann et al. 2012.
- Probabilistic: e.g.,
  - Schmidt and Rutland 2000: for spray combustion
  - DeVille et al. 2011 (Weighted Flow Algorithm): for aerosol dynamics. Implemented on PartMC (Riemer and West)
  - SDM
- Not a full list. No detailed comparison performed yet
- Accurate. **Less numerical diffusion.**
- **Cost could be smaller than Bin for higher dim.** (Detail follows)

5. Computational Cost of SDM

5.1. Asymptotic Behavior of SDM as $N_s \to N_r$

Scaling Law of Number Density of SDs $q(\xi, \boldsymbol{a}; N_s)$

Assuming that

$$q(\xi, \vec{a}, t; \alpha N_s) = \alpha^{k1} q(\alpha^{k2}\xi, \vec{a}, t; N_s)$$

Scaling law of this form exists

$$\sum_{\xi=0}^{\infty} \xi\, q(\xi, \vec{a}, t; N_s) = n(\vec{a}, t)$$

SDs expected to reproduce RD num density

$$\int d^d a \sum_{\xi=0}^{\infty} q(\xi, \vec{a}, t; N_s) = N_s \doteqdot const. \text{in time}$$

Conservation of N_s

$$\sum_{\xi=0,\alpha,2\alpha,..}^{\infty} = \frac{1}{\alpha} \sum_{\xi=0}^{\infty}$$

q is smooth enough with respect to ξ

Then, we can derive $(k_1,k_2) = (2,1)$, i.e.,

$$q(\xi, \vec{a}, t; \alpha N_S) = \alpha^2 q(\alpha\xi, \vec{a}, t; N_S)$$

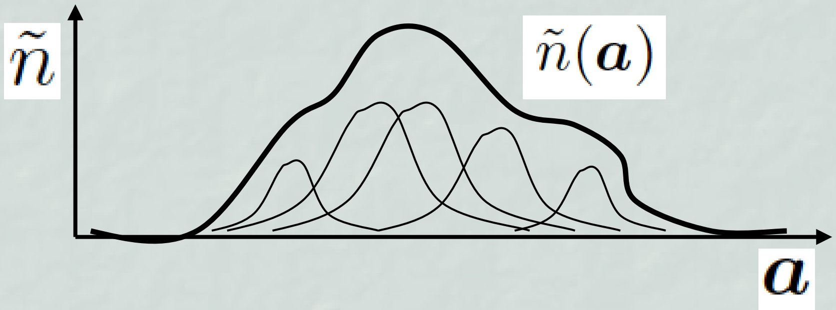
Scaling Relation Between Error and Cost

RD num density $n(\boldsymbol{a},t)$ can be estimated from SD population $\{(\xi_i,\boldsymbol{a}_i)\mid i=1,\ldots,Ns\}$. **Let's evaluate the error of this.**

Applying kernel density estimation (Terrell and Scott 1992),

$$\tilde{n}(\boldsymbol{a}) := \sum_{i=1}^{N_s} \xi_i W_\sigma^{(d)}(\boldsymbol{a}-\boldsymbol{a}_i).$$

$$W_\sigma^{(d)}(\boldsymbol{a}) := \frac{1}{(\sqrt{2\pi}\sigma)^d} \exp\{-\boldsymbol{a}^2/2\sigma^2\}.$$



Evaluate the error by Mean Integrated Squared Error (MISE)

$$C(\sigma) = E\left[\int d^d a\ \{n(\boldsymbol{a})-\tilde{n}(\boldsymbol{a})\}^2\right].$$

Combined with the scaling law of *q*, we can derive the relation between error *C(σ*)* and cost *Ns*

$$operation \sim N_s \sim \left(\frac{1}{\sqrt{C(\sigma^*)}}\right)^{(d+4)/2}, \qquad memory \sim N_s \sim \left(\frac{1}{\sqrt{C(\sigma^*)}}\right)^{(d+4)/2}.$$

Computational Cost of Bin method

Eulerian scheme to solve SCE separating $n(\boldsymbol{a},t)$ into grids.

Let the error of Bin method be $O(N_b^{-k})$

Then, we can derive

$$operation \sim N_b^{2d} \sim \left(\frac{1}{\sqrt{C}}\right)^{2d/k}, \qquad memory \sim N_b^{d} \sim \left(\frac{1}{\sqrt{C}}\right)^{d/k}.$$

here, C is the error defined by

$$C = \int d^d a \, \{n(\boldsymbol{a}) - n_b(\boldsymbol{a})\}^2 .$$

Comparison between SDM and Bin

If $d > \frac{4k}{4-k}$ and $k < 4,$ SDM is faster than Bin. (less operation)

If $d > \frac{4k}{2-k}$ and $k < 2,$ SDM needs less memory than Bin.

Exponential Flux Method (Bott 1998, 2000)

Numerically measured k is 1.5.

If d>2.4 SDM is faster, if d>12 SDM needs less memory.

Comment

- In general, in high dimensional space, random sampling is efficient than regular grid.
  - Regular grids have **"curse of dimensionality"**
  - Perhaps **"discrepancy"** of random sampling is lower in high dimension
- To derive the scaling of q, we didn't use any detail of SDM
  - **Similar analysis can be applied for any particle-based method**
- Cost is evaluated using the kernel density estimation method
  - Kernel density estimation itself is not part of SDM
  - **Maybe our analysis gives just a lower bound**

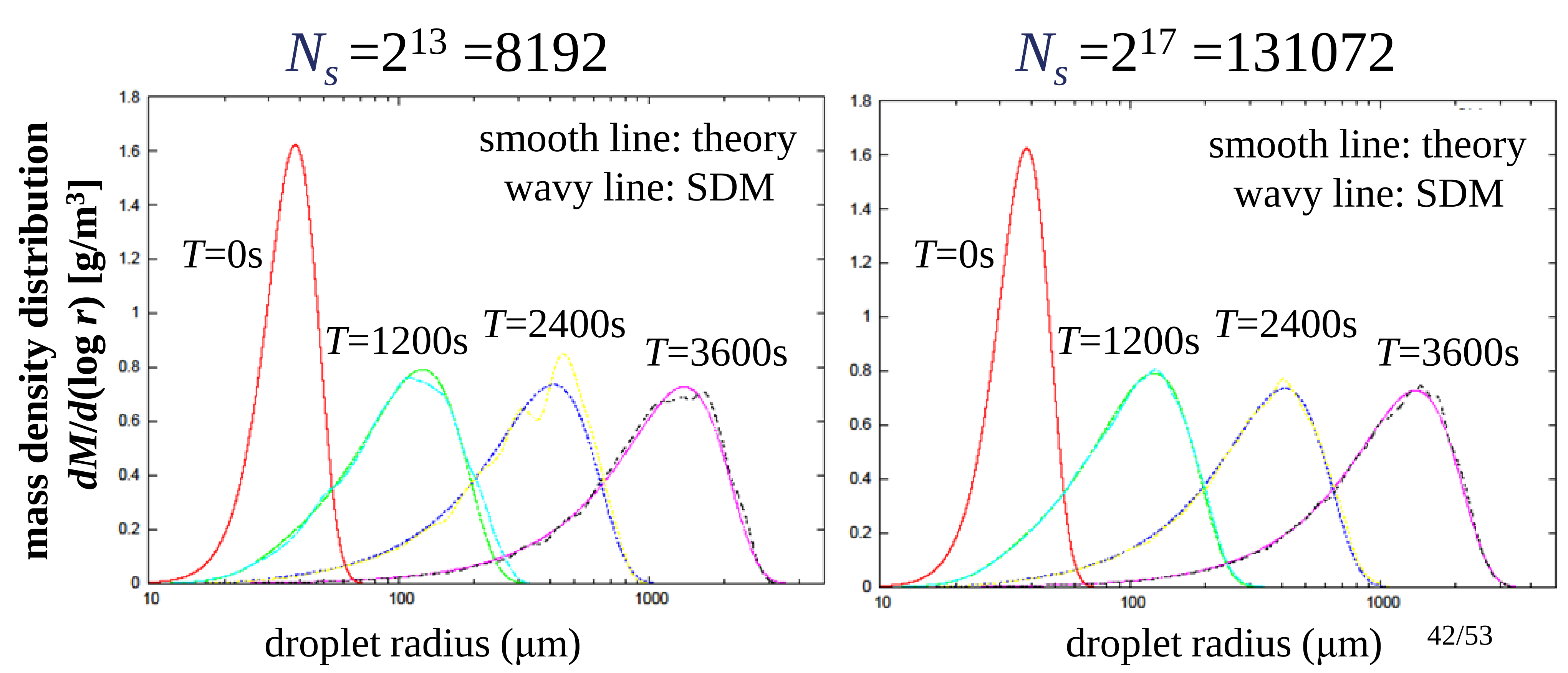
In practice, how many num of SDs are necessary??

5.2. Coalescence of Particles in a Small Box

Particles are confined to a small box and coalesce forever

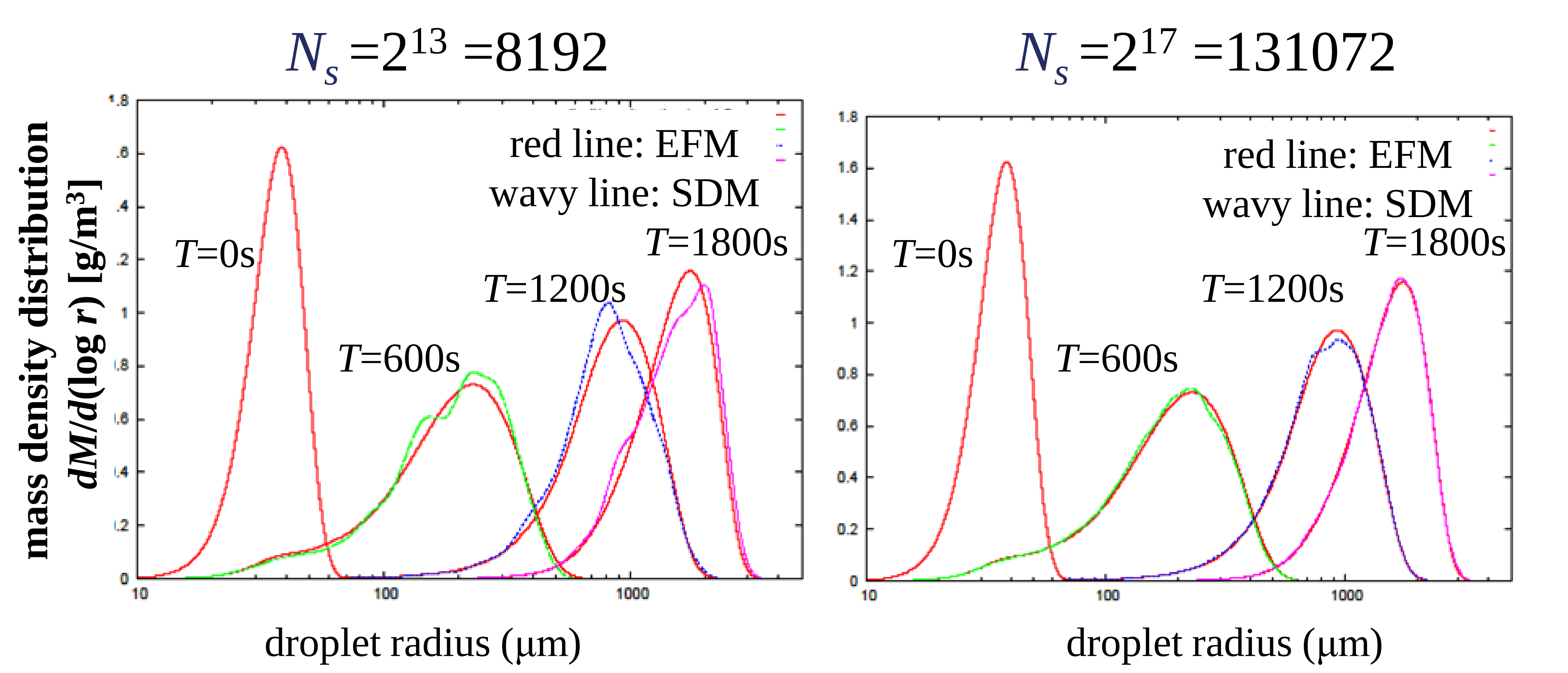
Golovin's Kernel

Analytical solution is known for this coalescence probability



Hydrodynamic Kernel (Initial Mean Radius <*r*0>=30um)

Much more realistic kernel for simulating clouds

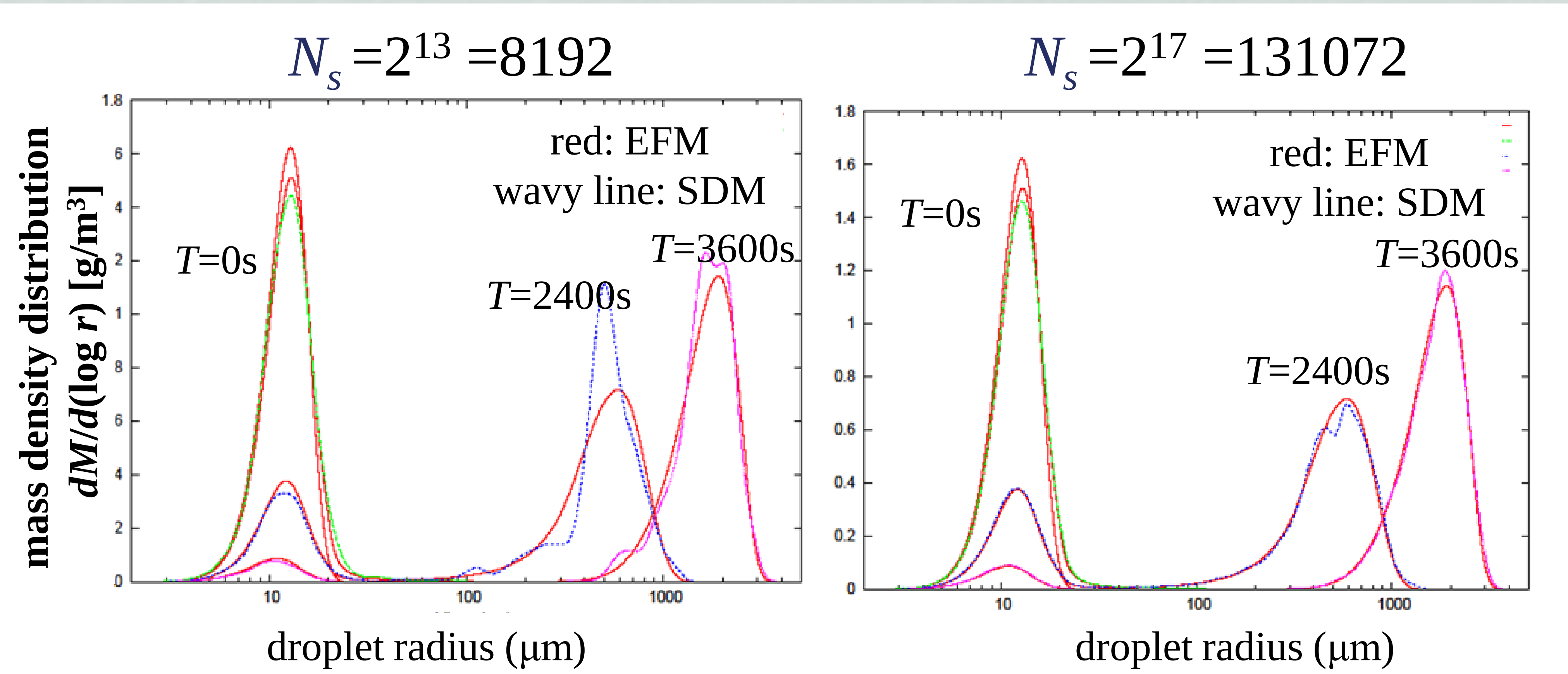


Hydrodynamic Kernel (Initial Mean Radius <*r*0>=10um)

Starting from a smaller size distribution

Coalescence seldom occurs, and two peaks are created

More difficult to simulate



Comments

8000 SDs could be sufficient for *d*=1?

There are arbitrariness how to initialize SDs

This time we used "uniform sampling" method

- Initialize SDs uniformly from [log r_{min}, log r_{max}] , and assign a multiplicity as follows

$$\xi_i = \frac{n_0(\log r_i)\log\left(r_{\mathrm{max}}/r_{\mathrm{min}}\right)}{n_s}$$

here $n_s = N_s/\Delta V$, $n_0(\log r)$: initial num density of RDs

- This reduces sampling error and improve the convergence

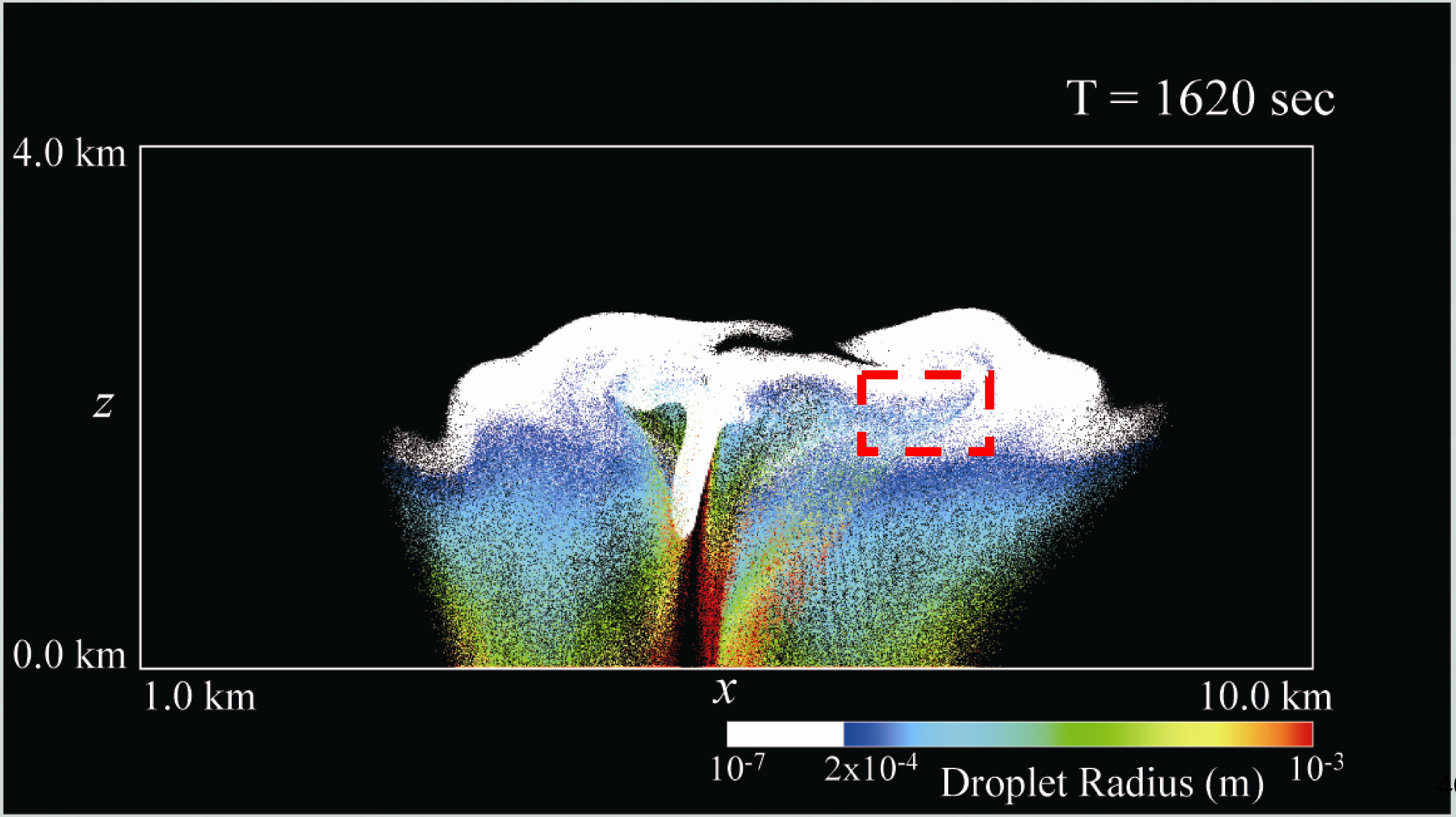
In S.S. et al (2009) we employed "constant multiplicity" method.

- This would not be recommended.

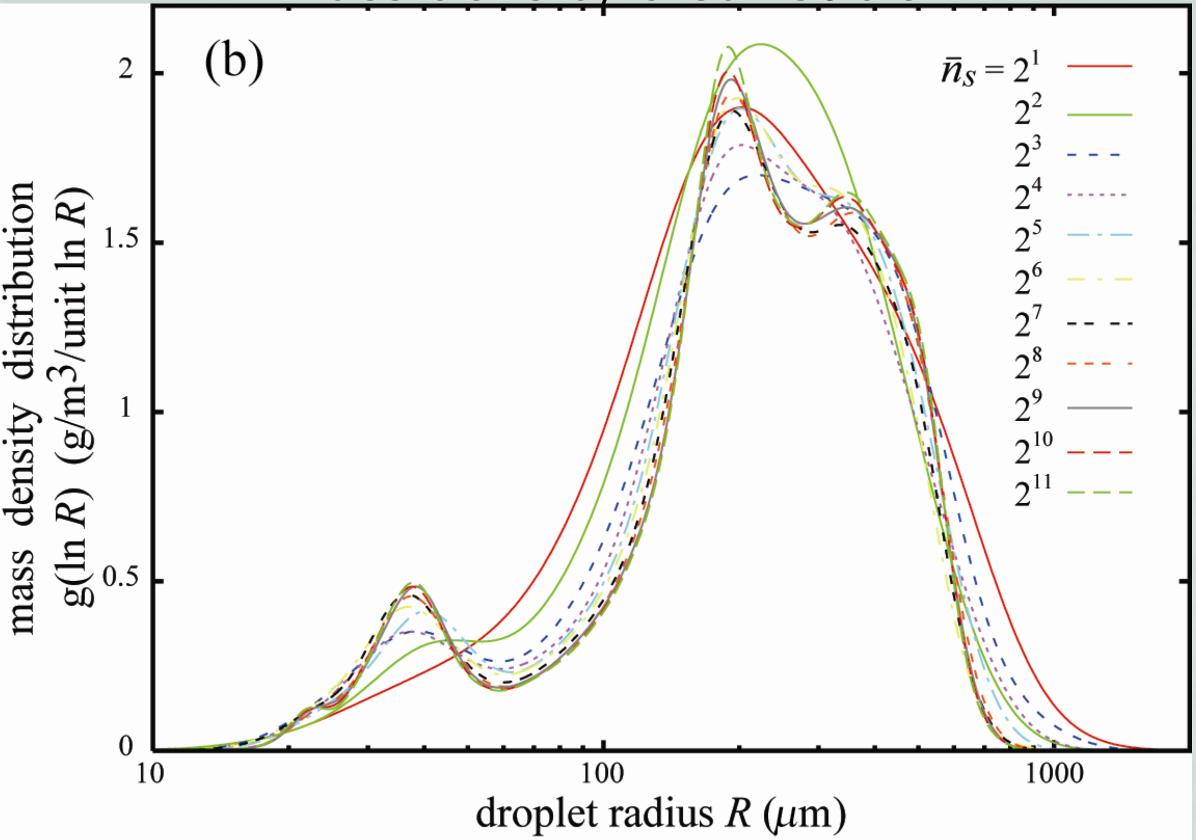
5.3. Isolated Shallow Cumulus (2D, 30min)

Initially Very Clean Case ($10^7/m^3$)

Particle size distribution in the square region and precipitation amount are investigated for various SD num



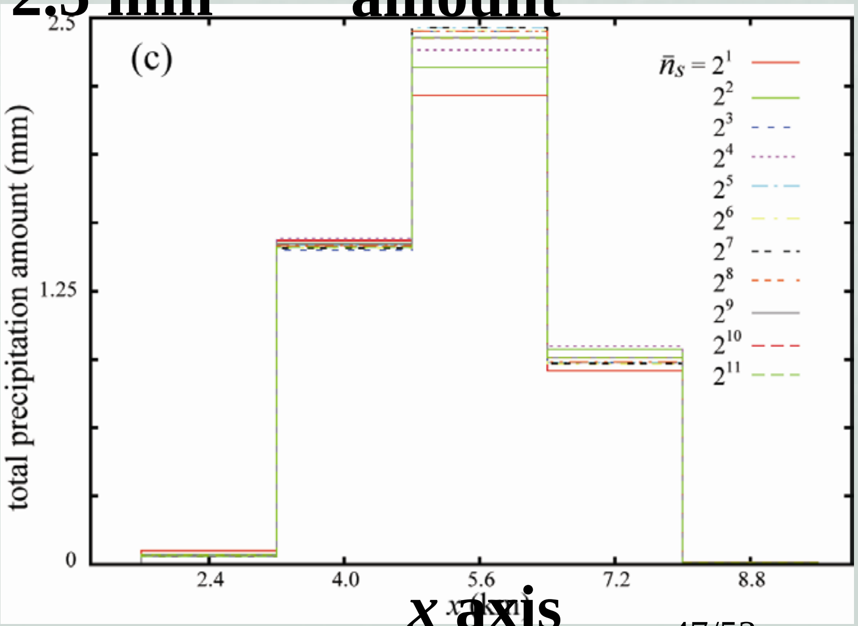
mass density distribution



initial number density of NaCl aerosol
n=10^7/m^3

accumulated precipitation amount

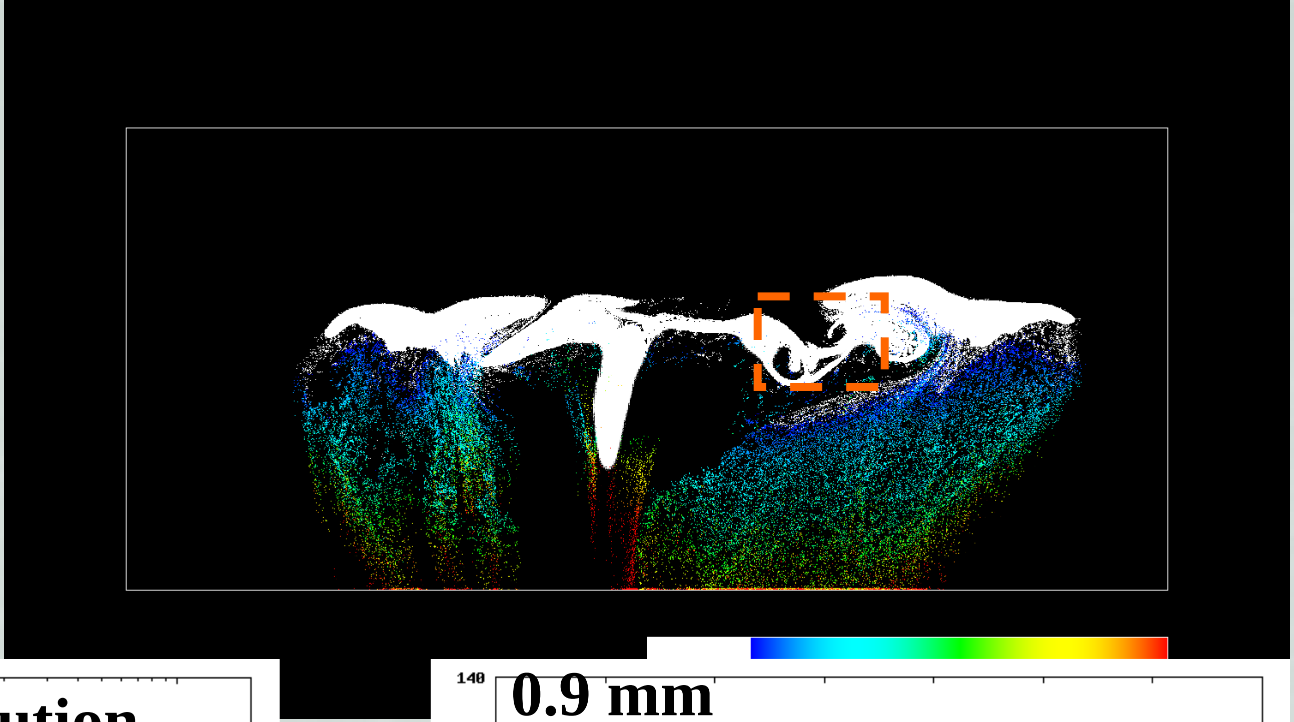
2.5 mm

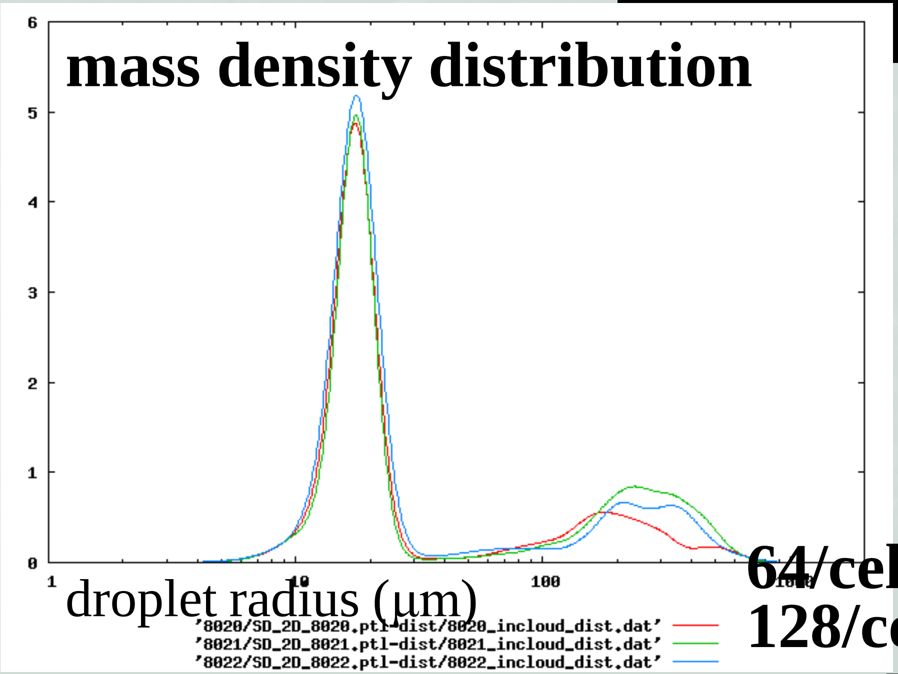


x axis

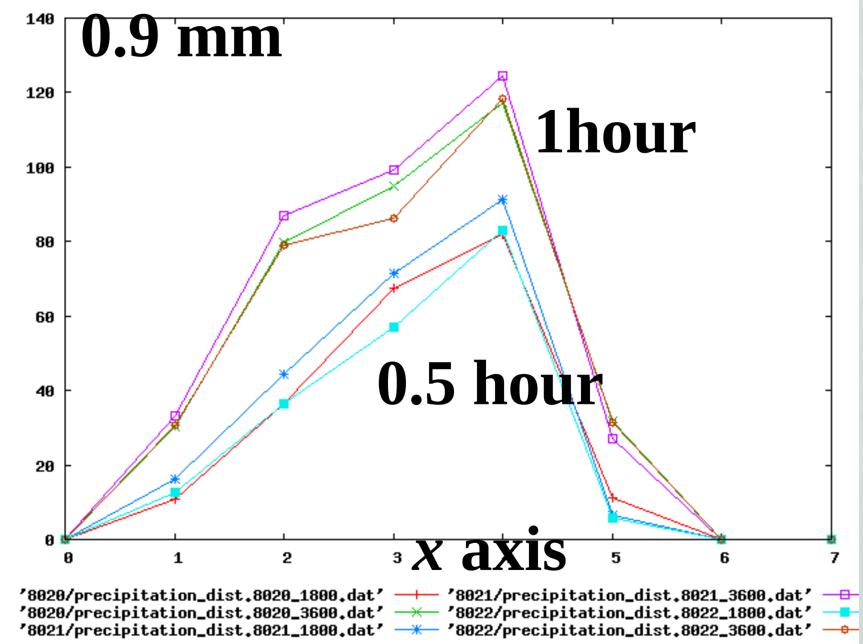
Good numerical convergence at SDs #32/cell

Initially clean case
NaCl aerosol
n=10^8/m^3

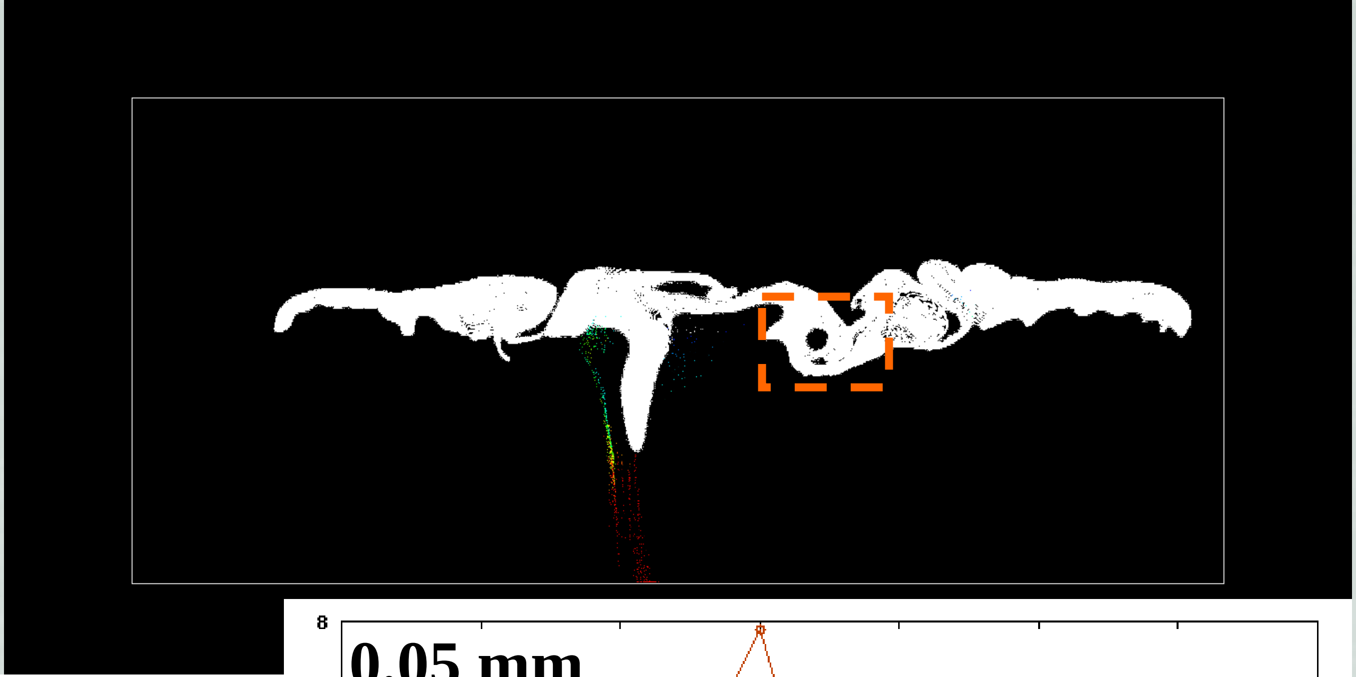


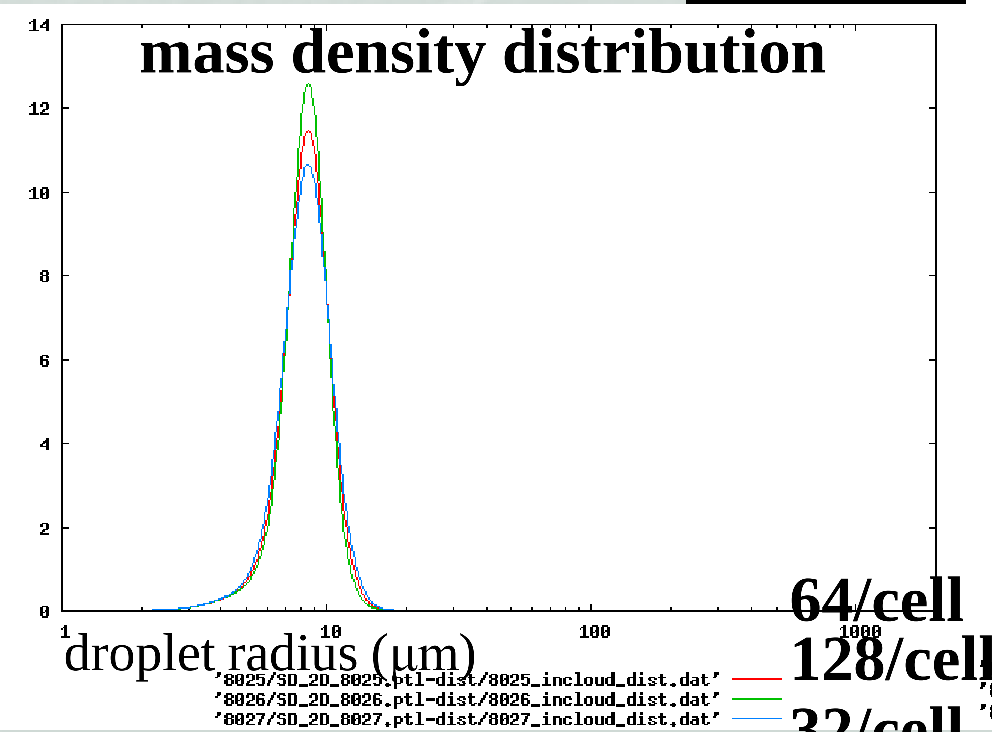


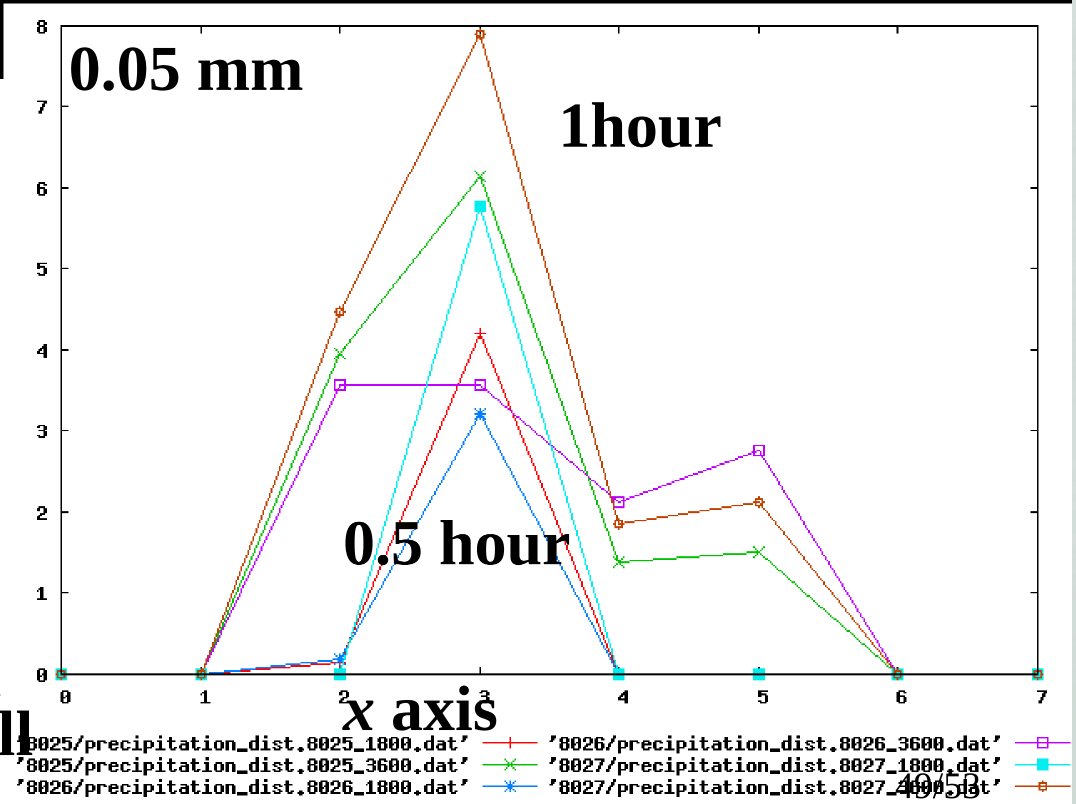
64/cell
128/cell
32/cell



Initial polluted case
NaCl aerosol
$n=10^9/m^3$



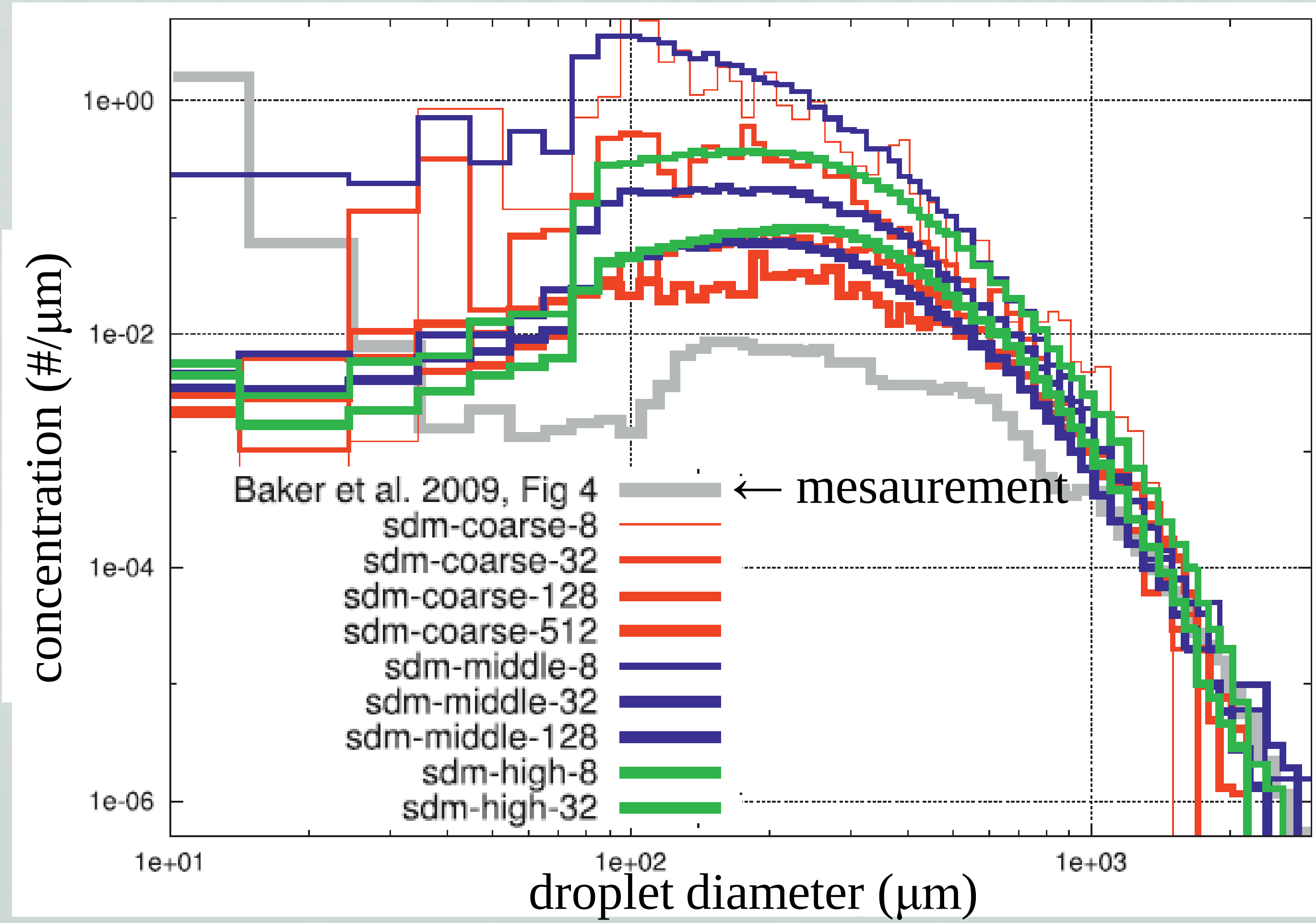




5.4. Shallow Trade Wind Cumuli Field (3D, 24h)

Simulation of precipitating cumuli field is performed based on RICO setup (Arabas and Shima, 2011)

Rain droplet size distribution below cloud based



6. Concluding Remarks

Summary

SDM is particle-based and probabilistic cloud microphys model

Coalescence is solved by a new Monte Carlo scheme

conservation of N_s , $O(N_s)$ cost, robust to large Δt

Computational cost of SDM is discussed

Asymptotically, SDM could be faster than Bin when $d \geqq 3$

In practice, if d=2,

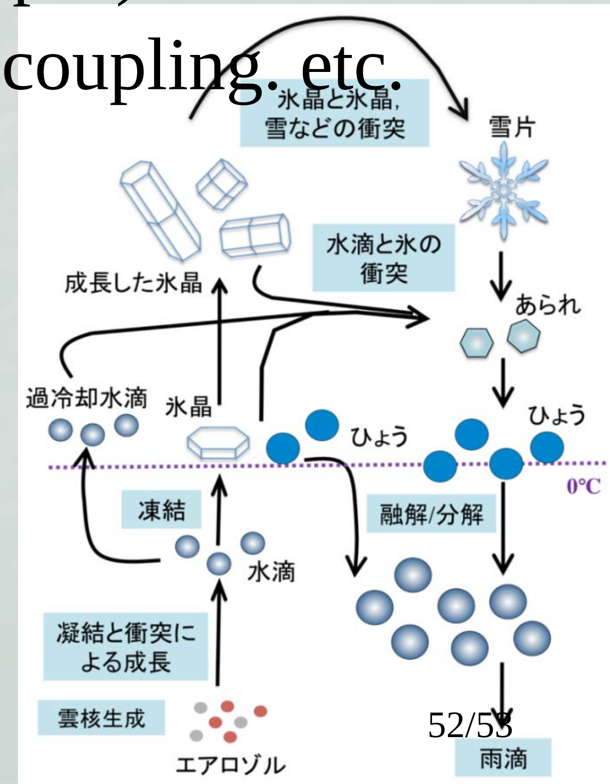
Even SDs #8/cell can produce a qualitative results,

SDs at least #64/cell to at most #8000/cell produce a quantitative results

Suitable for simulating detailed cloud microphysics, e.g., aerosol-cloud interaction

Future Direction

- Numerical convergence
  - Dependency on Δt and the spatial resolution of fluid
  - Comprehensive study is ongoing with Y.Sato (RIKEN)
- Improvement of the algorithm
  - "Multiple coalescence" can be improved to make it more robust to large Δt. (1000 times speedup??)
  - Breakup. Redistribution of SDs. Vapor coupling. etc.
- Ice phase
  - Goal of this year
- Atmospheric chemistry
  - In few years. (with a postdoc)
- Turbulence effect
  - Sub-grid scale vapor fluctuation, etc.



Thank you for your attention!

Co-workers

Cloud Modeling and Simulations

K. Hasegawa (Chuden CTI Co. Ltd.)
Y. Sato (RIKEN)
S. Arabas (Warsaw Univ.)
K. Kusano (Nagoya Univ./JAMSTEC)
A. Sakakibara (Chuden CTI Co. Ltd.)
K. Tsuboki (Nagoya Univ./JAMSTEC)
W. Ohfuchi (JAMSTEC)

Data Processing and Visualization

F. Araki (JAMSTEC)
S. Kawahara (JAMSTEC)

Ice Phase Physics

Y. Sato (RIKEN)
A. Hashimoto (MRI)

Atmospheric Chemistry

M. Kajino (MRI)
M. Deushi (MRI)
Y. Sato (RIKEN)