Super-Droplet Method (and its Application to Mixed-Phase Clouds)

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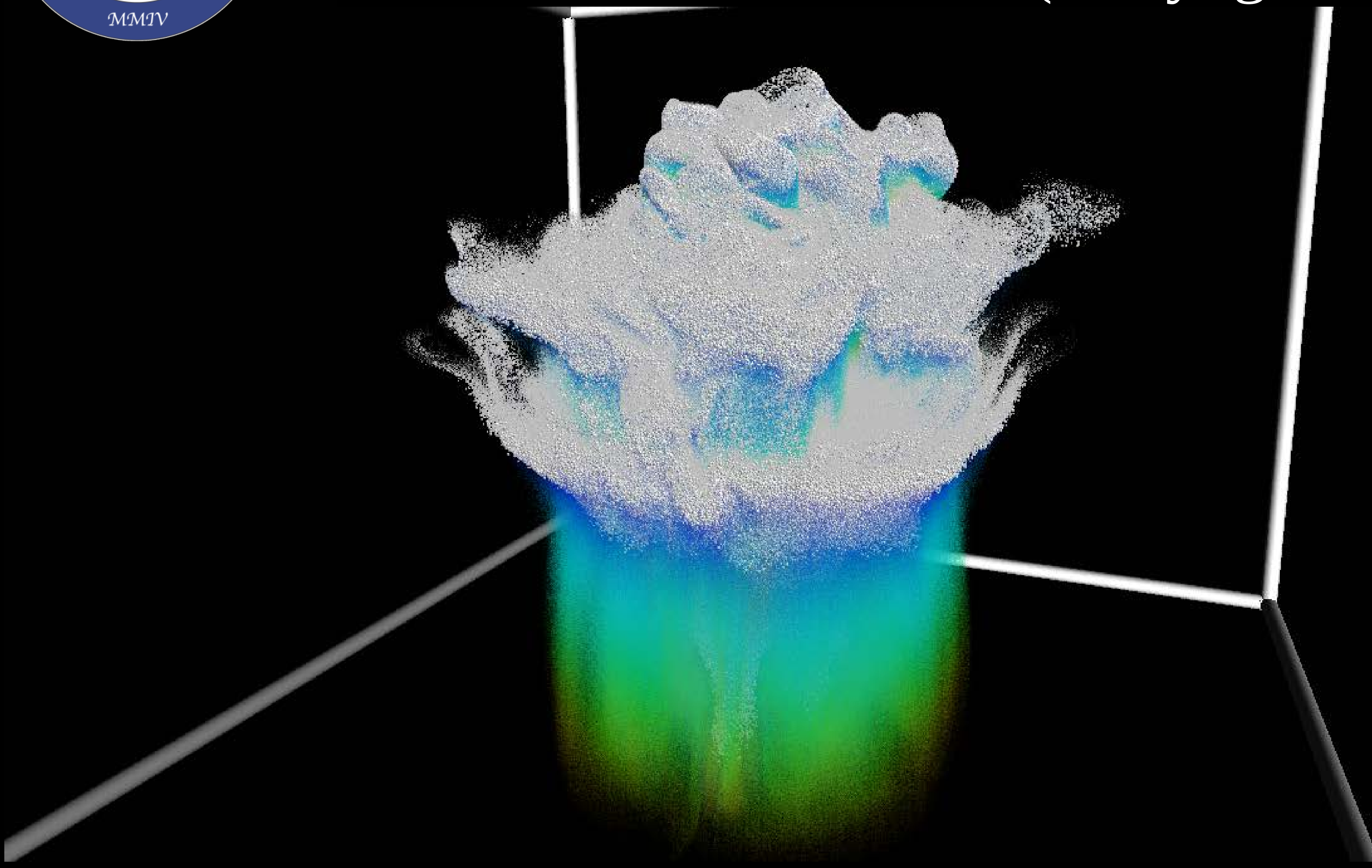


Abstract

Super-Droplet Method (SDM) is **a particle-based scheme to simulate cloud-microphysics accurately.** (S.S. et al. 2009)

Basic framework, advantages, and future directions of SDM will be presented

Contents

1. Motivation: It is still difficult to simulate clouds accurately

Cloud Dynamics

dry air, vapor, trace gas.

interaction

Cloud Microphysics

particles (aerosol/cloud/precipitation)

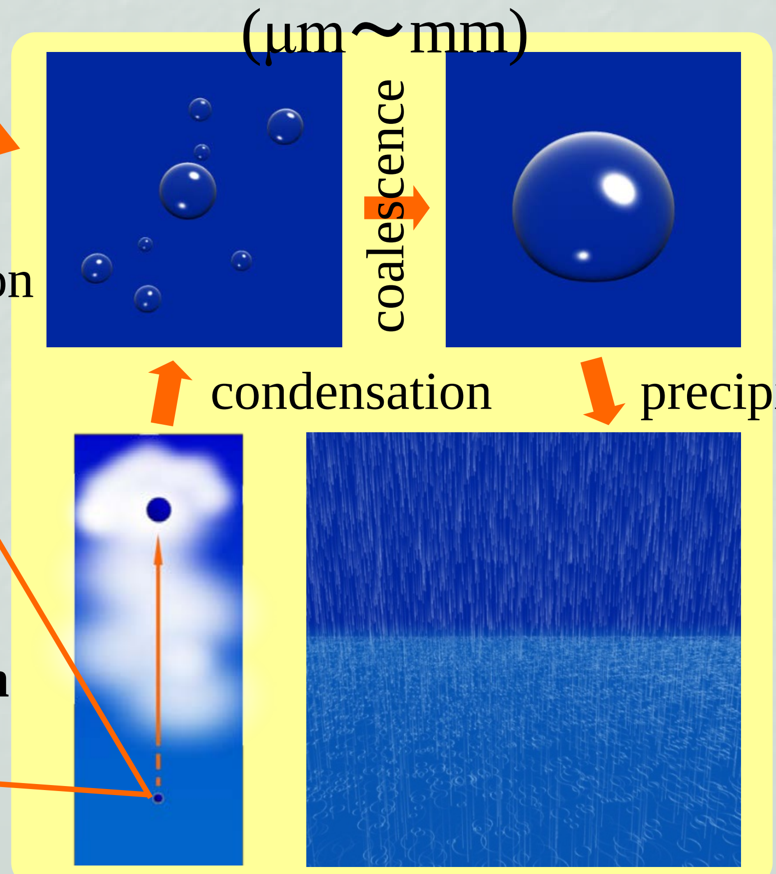
nucleation from gases
or rolling up of dusts

chemical
reactions

aerosol particles

evaporation

**cloud-
aerosol
interaction**



Aerosol particles

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2. Basic Equations of Clouds and their Hierarchy

2.1 Hierarchy of Description of Cloud Microphysics

	Cloud Microphysics		Analogy in Fluid Dynamics
micro	**Droplet dynamics with deterministic collision-coalescence**		**Molecular dynamics with deterministic collision**
	↓ well-mixed ansatz		↓ molecular chaos ansatz
meso	SDM: **Droplet dynamics with stochastic collision-coalescence**		**Molecules dynamics with stochastic collision**
	↓ decoupling assumption		↓ decoupling assumption
	Smoluchowski eq. (Number density dynamics)		**Boltzmann eq. (Number density dynamics)**
	⇣ semi-empirical		↓ local equilibrium
macro	**bulk model (closure in lower moments)**		**Navier-Stokes eq. (closure in lower moments)**

2.2. Mesoscopic Description of Cloud Microphysics

Introduce the basic equations of particles with stochastic coalescence (but no breakups)

Then, also derive the Smoluchowski eq.

State variables

Particles (or Droplets): generic name for aerosol/cloud/precipitation particles

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

$\boldsymbol{a}(t)=\{a^{(1)}(t), a^{(2)}(t), \ldots, a^{(d)}(t)\}$: the state of a 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.

Stochastic Coalescence of particles

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 ΔV have some possibility to coalesce

In general C and K also depend on fluid field

These are the mesoscopic basic equations of cloud microphysics

Another mesoscopic representation follows.

Smoluchowski eq. (Stochastic Coalescence Equation; SCE)

Let $n(\boldsymbol{a},\boldsymbol{x},t)$ be the number density of particles at time t, at $\boldsymbol{x}$, with attribute $\boldsymbol{a}$. **Under the 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., we can derive

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

Here, $\boldsymbol{a}' \rightarrow\leftarrow \boldsymbol{a}'' = \boldsymbol{a}$.

Decoupling in not valid if the well-mixed volume is small

2.3. 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 $\boldsymbol{v}$, 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

$\rightarrow$ 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,

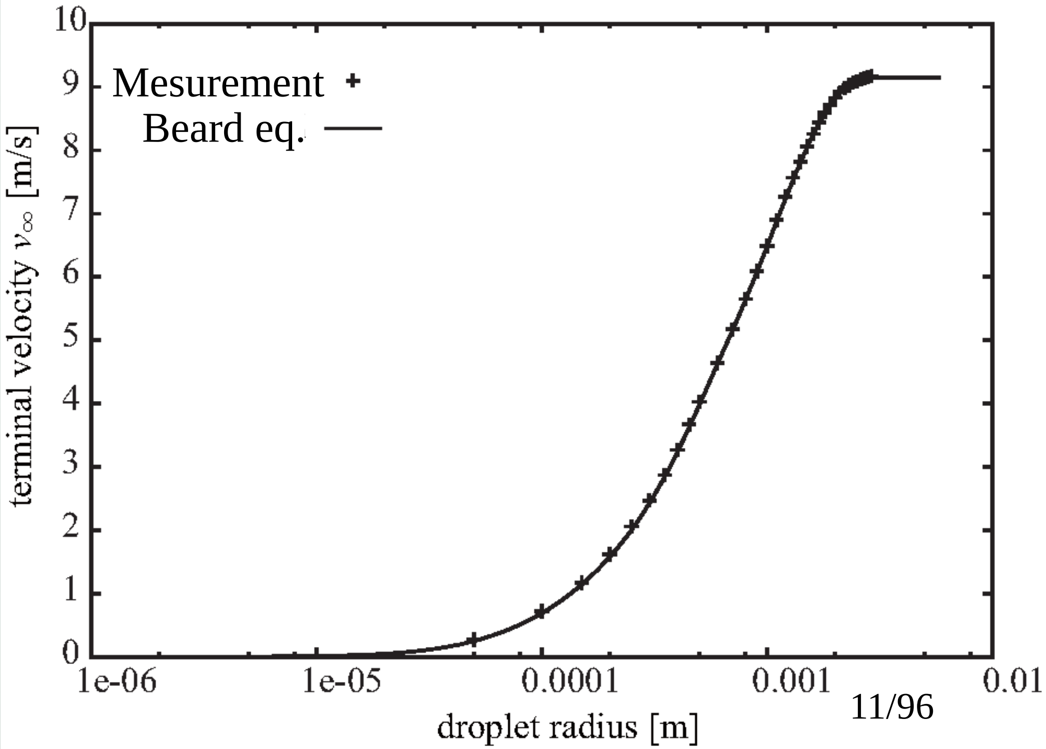
$$\boldsymbol{v}_i(t) = \boldsymbol{U}_i^* - \hat{\boldsymbol{z}} v_\infty(R_i, T_i^*, P_i^*), \quad d\boldsymbol{x}_i/dt = \boldsymbol{v}_i,$$

$\boldsymbol{U}_i^*$, 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

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

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

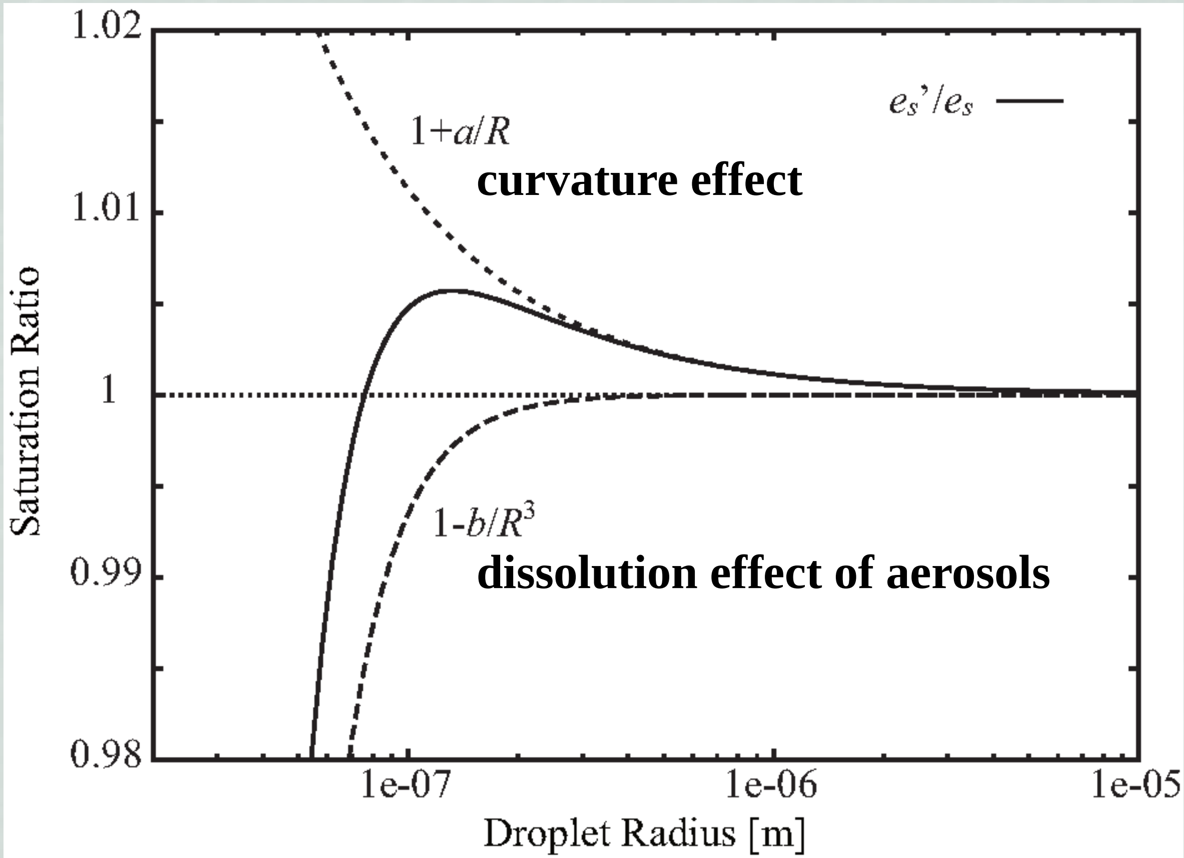
$$F_k(T_i^*) = \left(\frac{L}{R_v T_i^*} - 1 \right) \frac{L \rho_{\mathrm{liq}}}{K T_i^*}, \quad F_d(T_i^*) = \frac{\rho_{\mathrm{liq}} R_v T_i^*}{D e_s(T_i^*)}.$$

…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

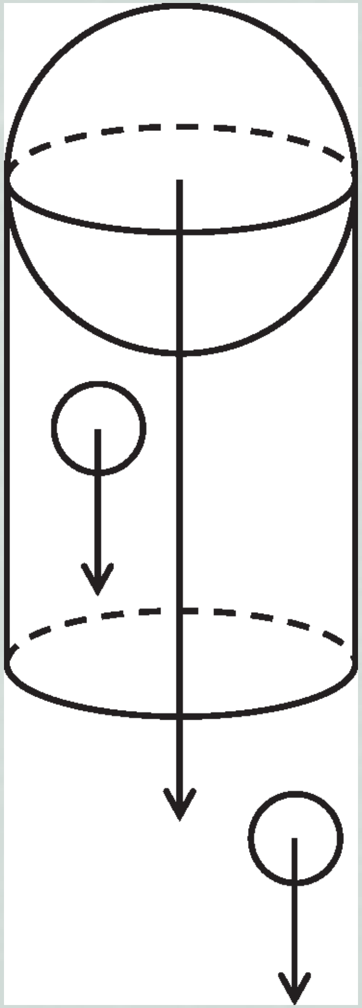
Consider two particles j and k in a volume ΔV

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 ratio of sweep volume and ΔV

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

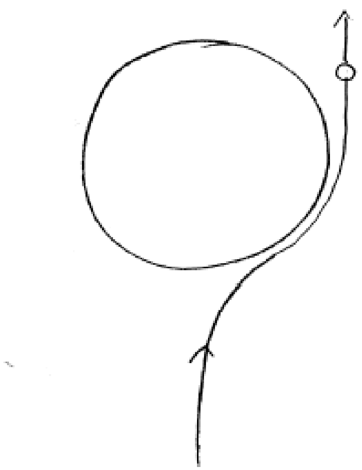


However,

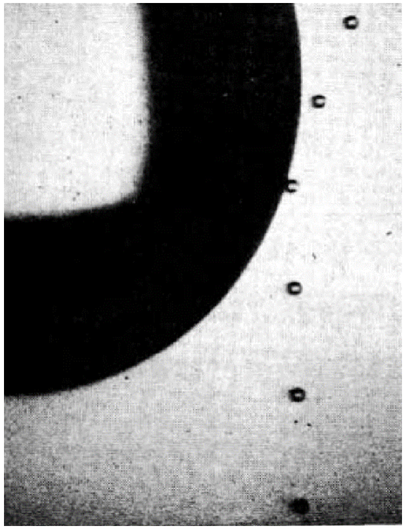
…cont. (Coalescence of particles by the gravitational settling)

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 $E(R_j, R_k)$

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

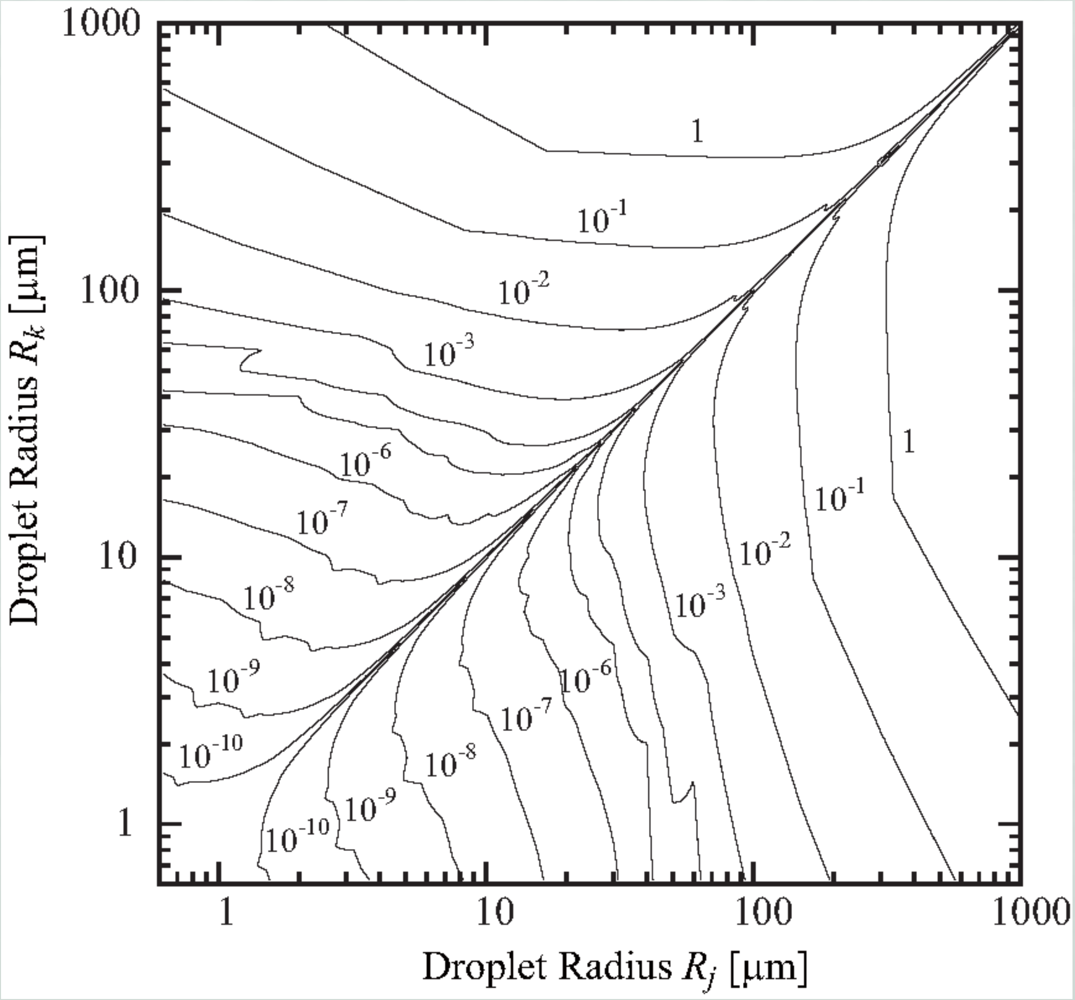
e.g., theories of Davis(1972), Jonas(1972), Hall(1980)

…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°C.

- 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)



2.4. 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

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

density of liquid water / unit space volume

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

$\rho = \rho_d + \rho_v$: 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

3. Super-Droplet Method

Mesoscopic governing equation of the cloud microphysics

Dynamics of particles with stochastic coalescence

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

$$P_{jk} = K(\boldsymbol{a}_j, \boldsymbol{a}_k)\Delta t/\Delta V.$$

Smoluchowski eq. (for number density of particles)

under decoupling assumption

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

SDM is a numerical scheme to solve this equation

For simulating clouds, we need to mutually couple SDM with an LES (Large Eddy Simulation) model

Here after, 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

Coalescence of SDs is also a stochastic event

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

SD # won't be decreased after the coalescence

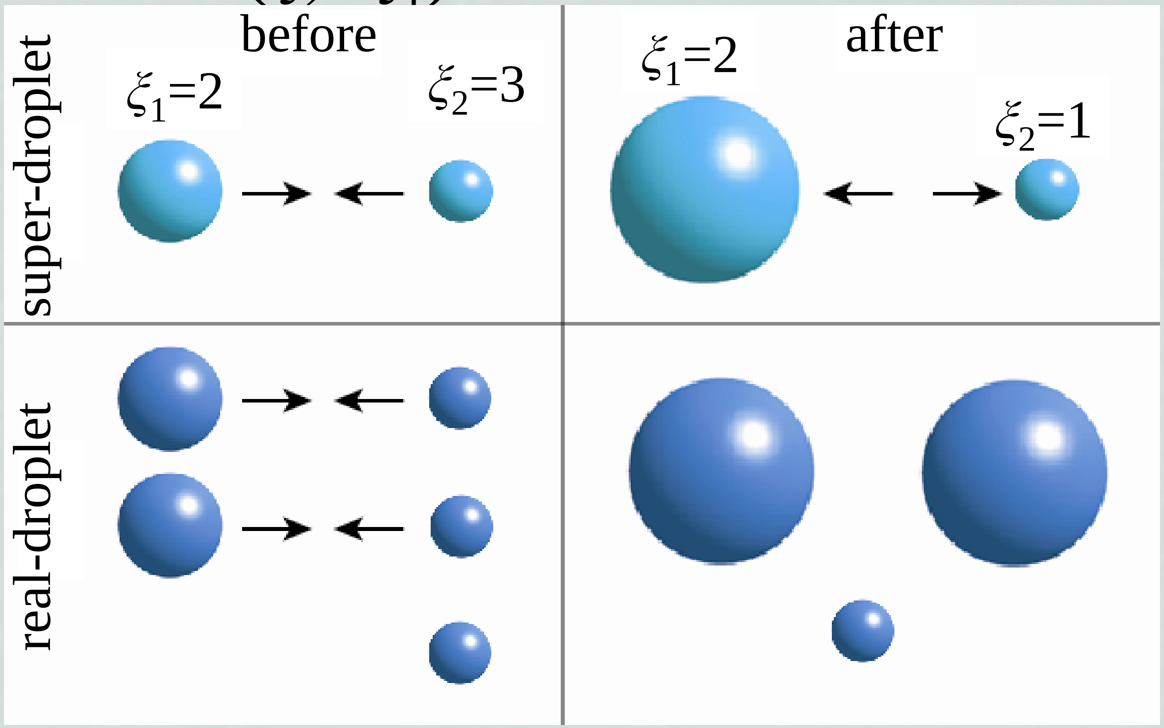
The expected results is consistent with RD

(Detail follows)

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

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

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

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

3.2. Numerical Implementation of the SDM

Outlook

Cloud microphysics (= Super-Droplet Method)

Individual dynamics

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

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

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

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

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

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

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)

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

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

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

(also update fluid)

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

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 ${}_{N_s'}C_2$ 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

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

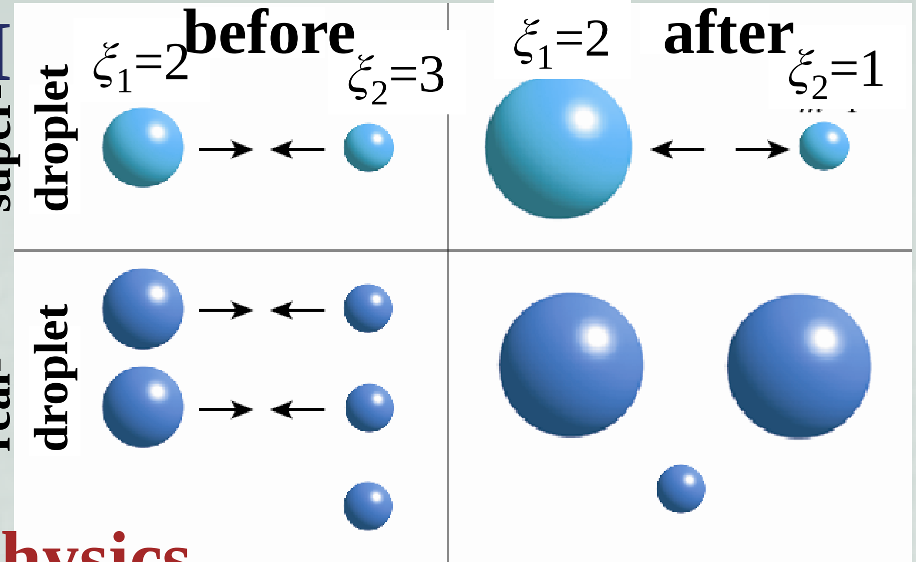
Coalescence occurs q times

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

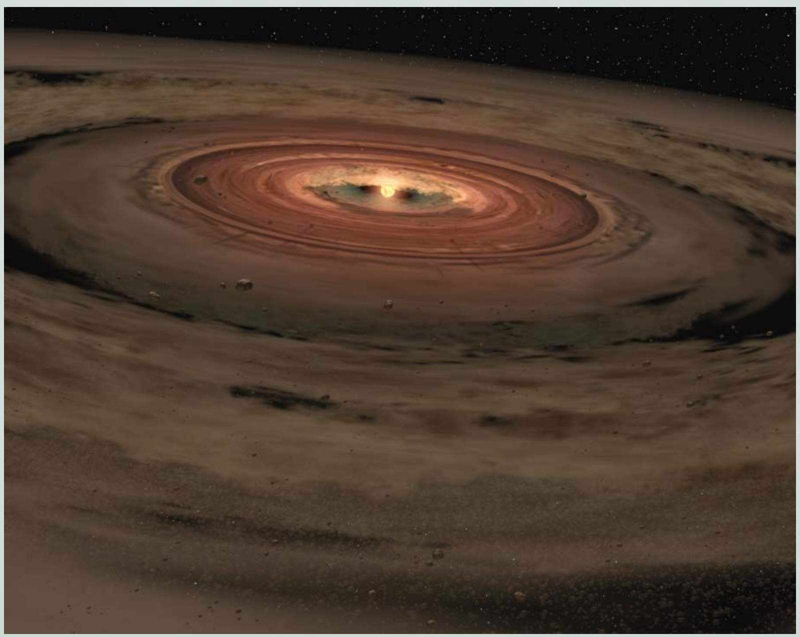
This makes our method robust to large Δt_c

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

3.3. Characteristics of the SDM



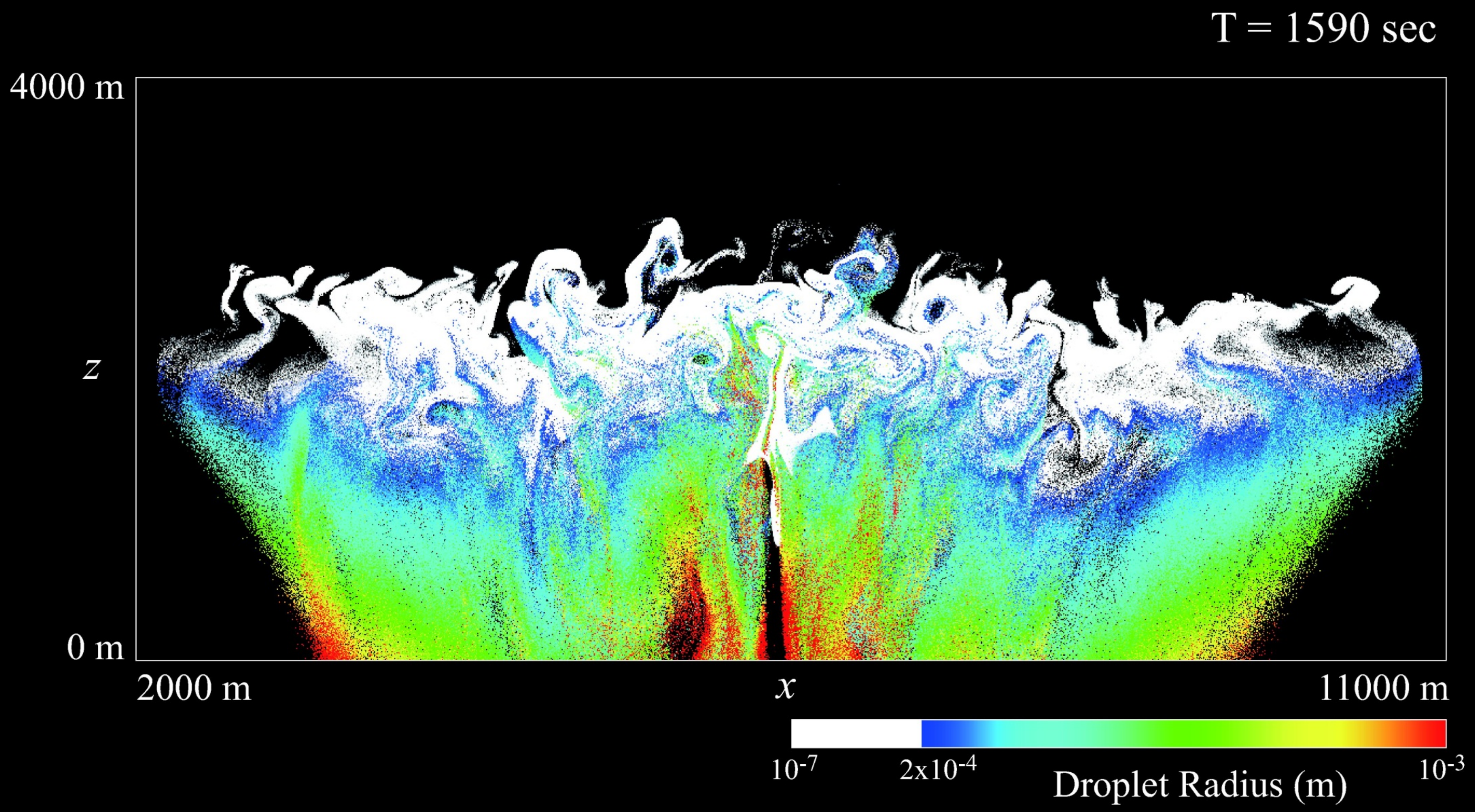
- Super-Droplet represents multiple number of real particles
- **Original Monte Carlo scheme for coalescence**
- **Suitable for detailed cloud microphysics**
- Applicable if particles collide and coalesce repeatedly



Star formation, Spray combustion, bubbles, volcanic fumes, population dynamics etc.

Protoplanetary disk (imaginary. from NASA HP)

4. Demonstration (Isolated shallow cumulus, 2D)



Shallow cumulus (3D, Δz= 8 m)

grid: 624x1024x1024, particles: #10^10,

ES 256 nodes

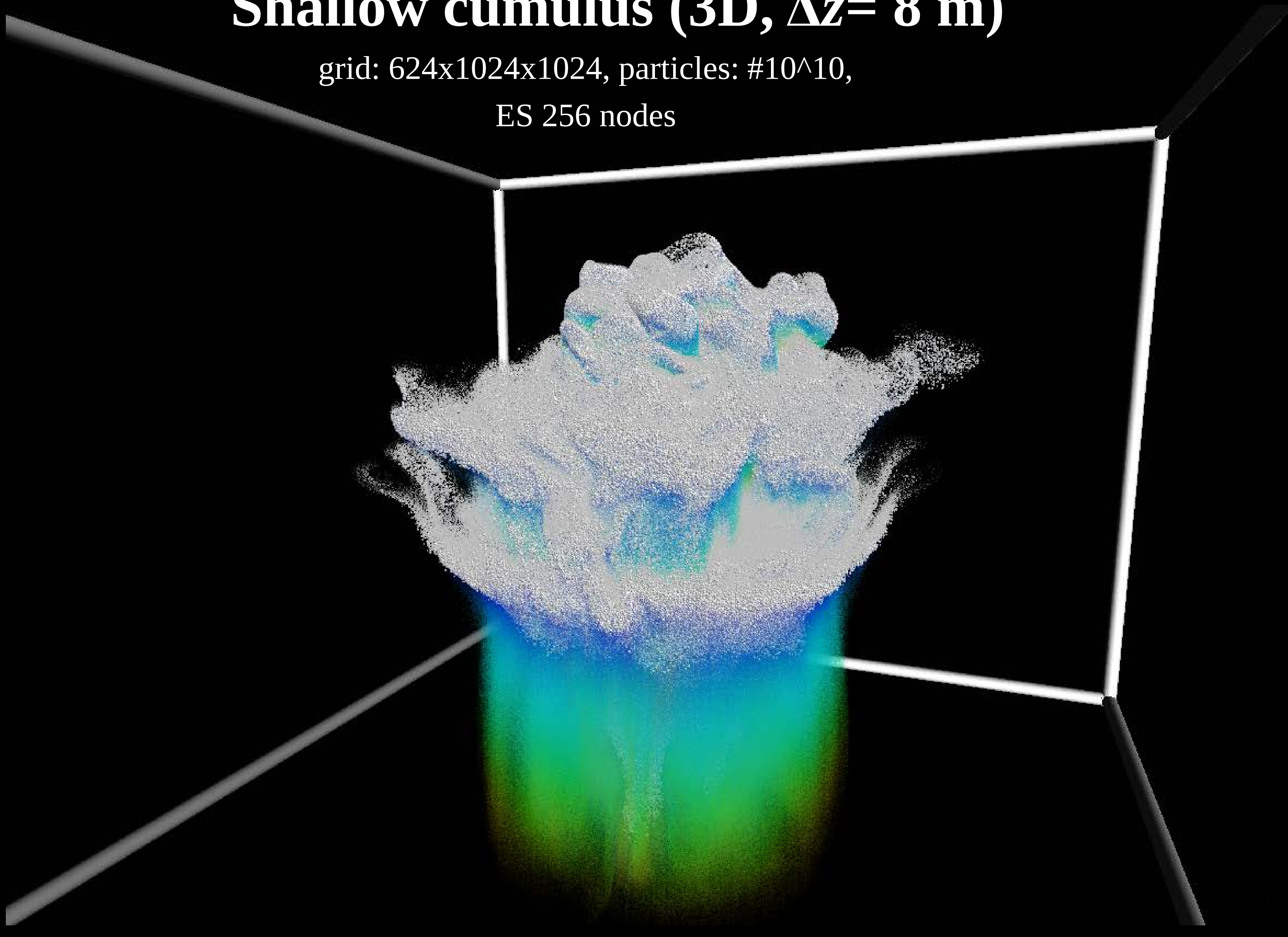
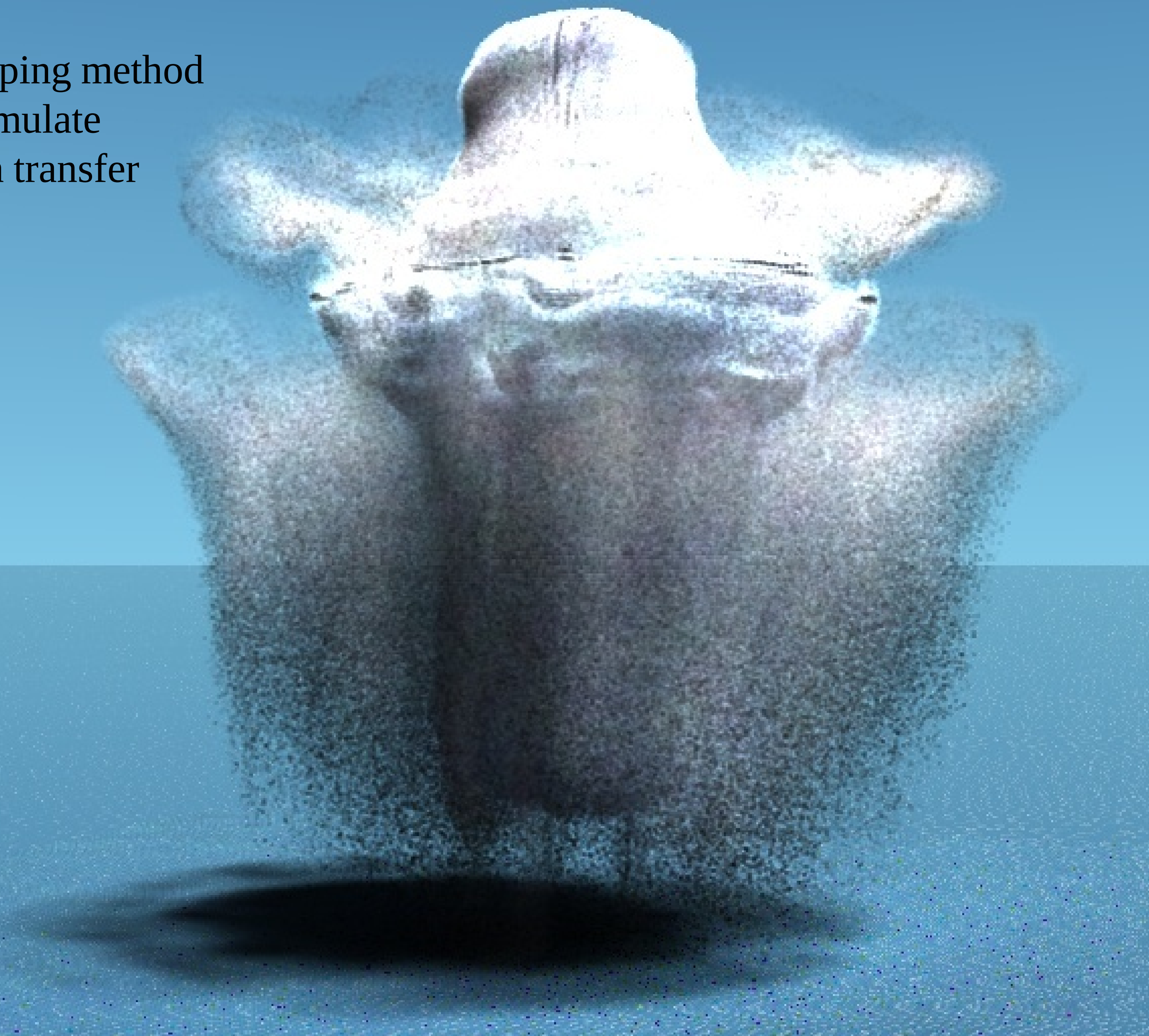


photo realistic visualization:

Δz= 16 m

Photon-mapping method
is used to simulate
the radiation transfer



5. Computational Cost of SDM

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

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

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.,

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

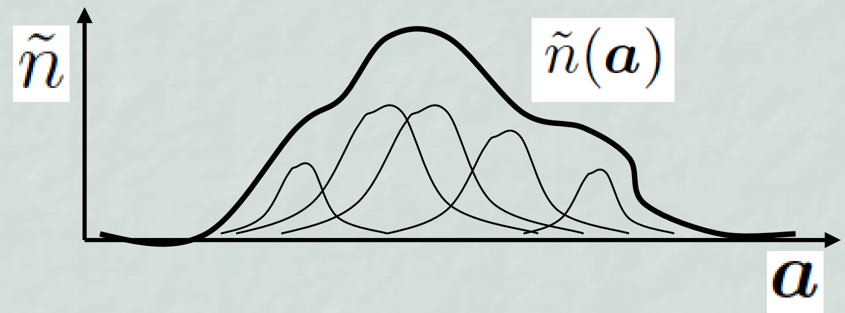
Scaling Relation Between Error and Cost

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*

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

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??

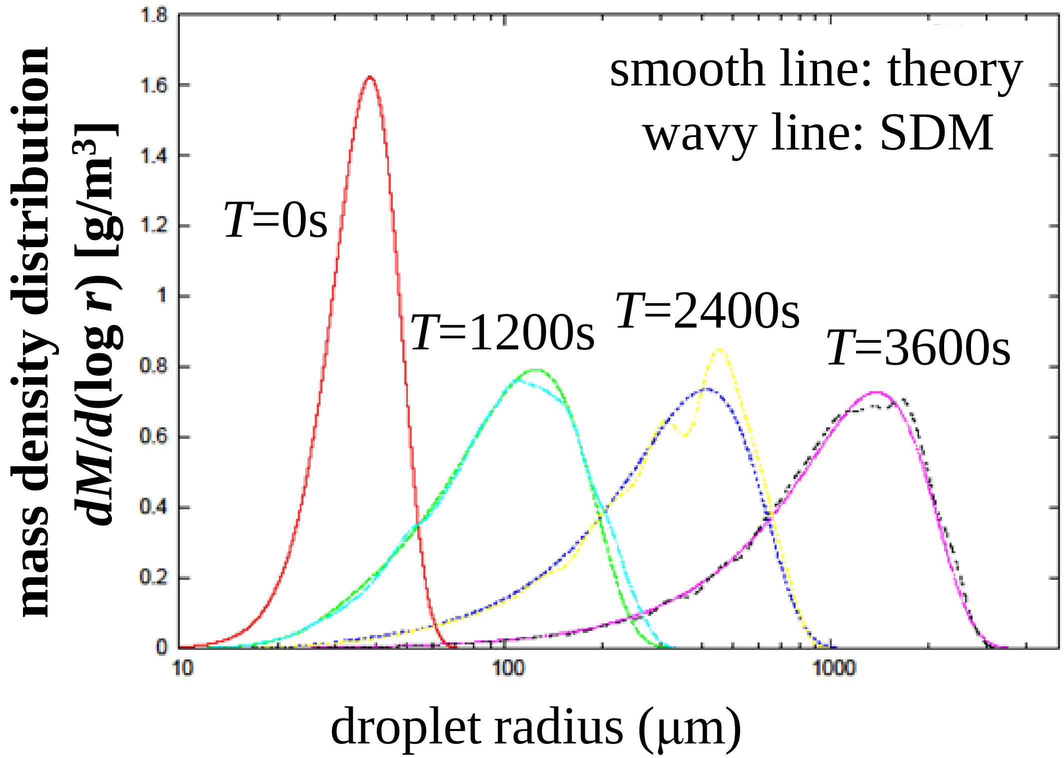
5.2. Coalescence of Particles in a Small Box

Particles are confined to a small box and coalesce forever

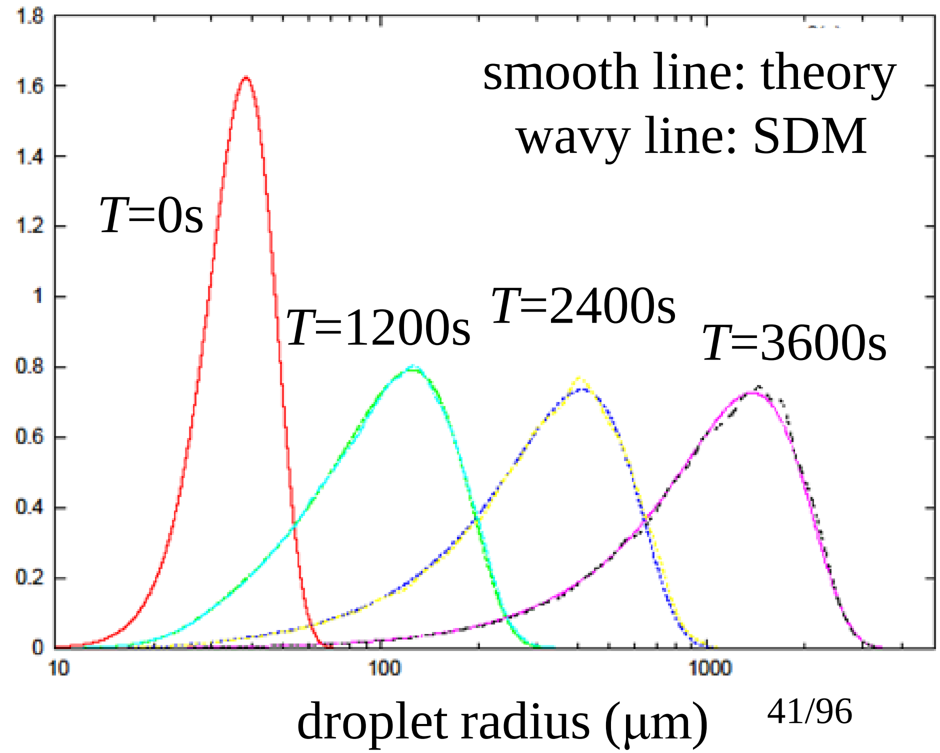
Golovin's Kernel

Analytical solution is known for this coalescence probability

$N_s = 2^{13} = 8192$

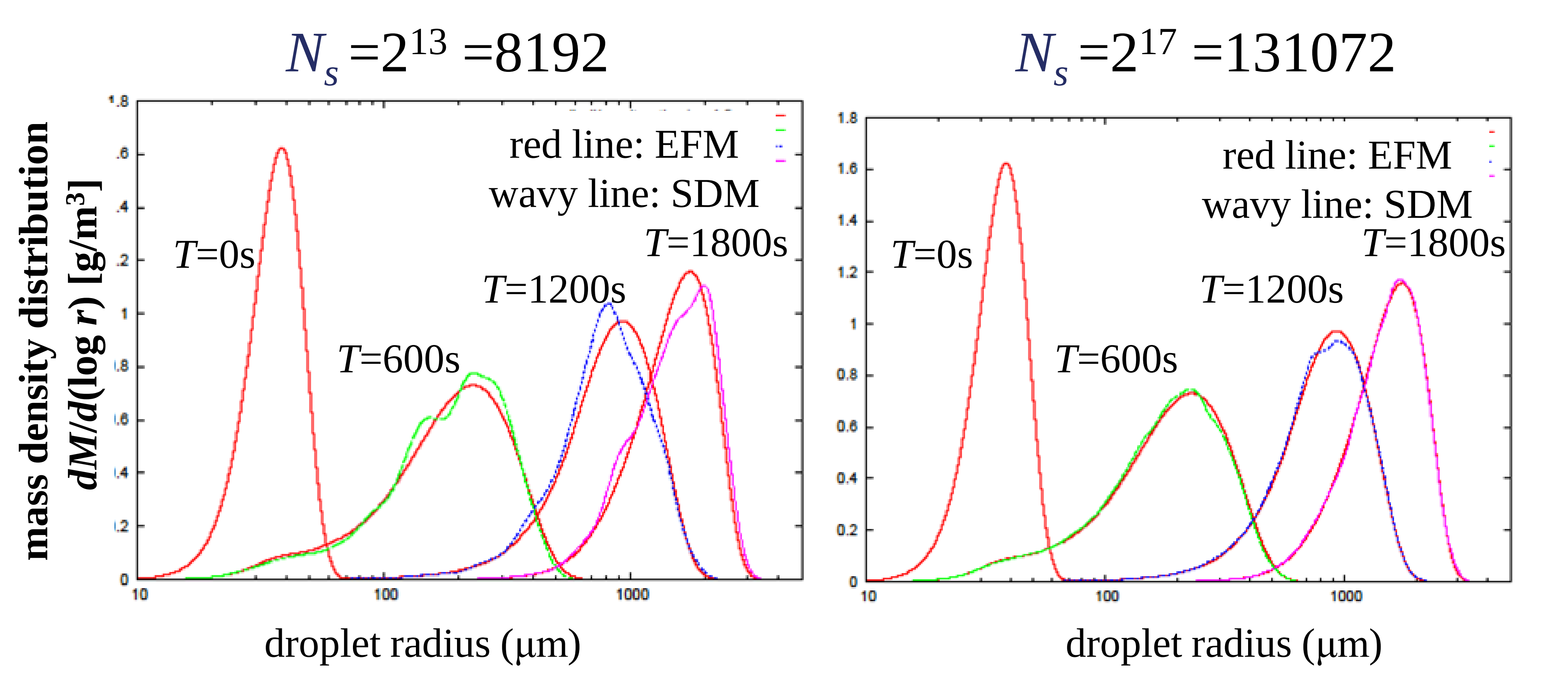


$N_s = 2^{17} = 131072$



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

Much more realistic kernel for simulating clouds

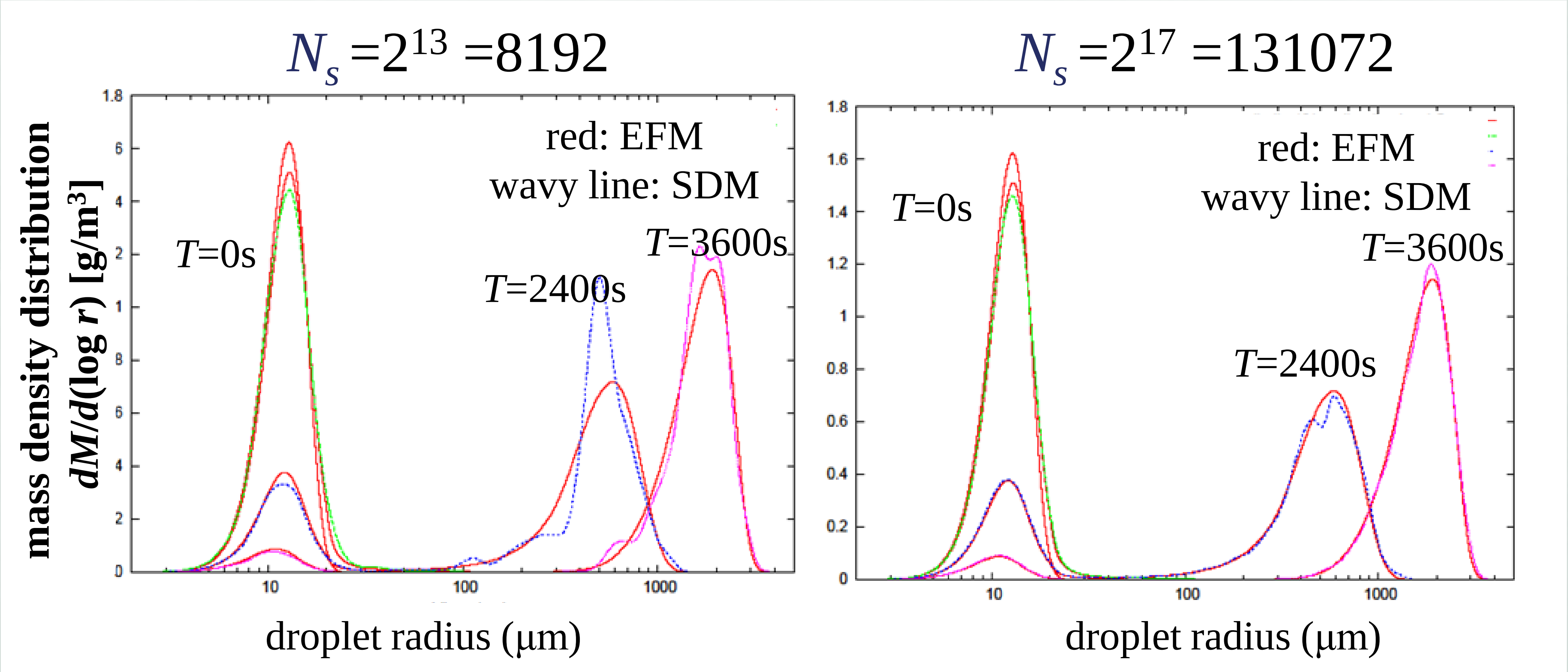


Hydrodynamic Kernel (Initial Mean Radius <*r*0>=10um)

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

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

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

This reduces sampling error and improve the convergence

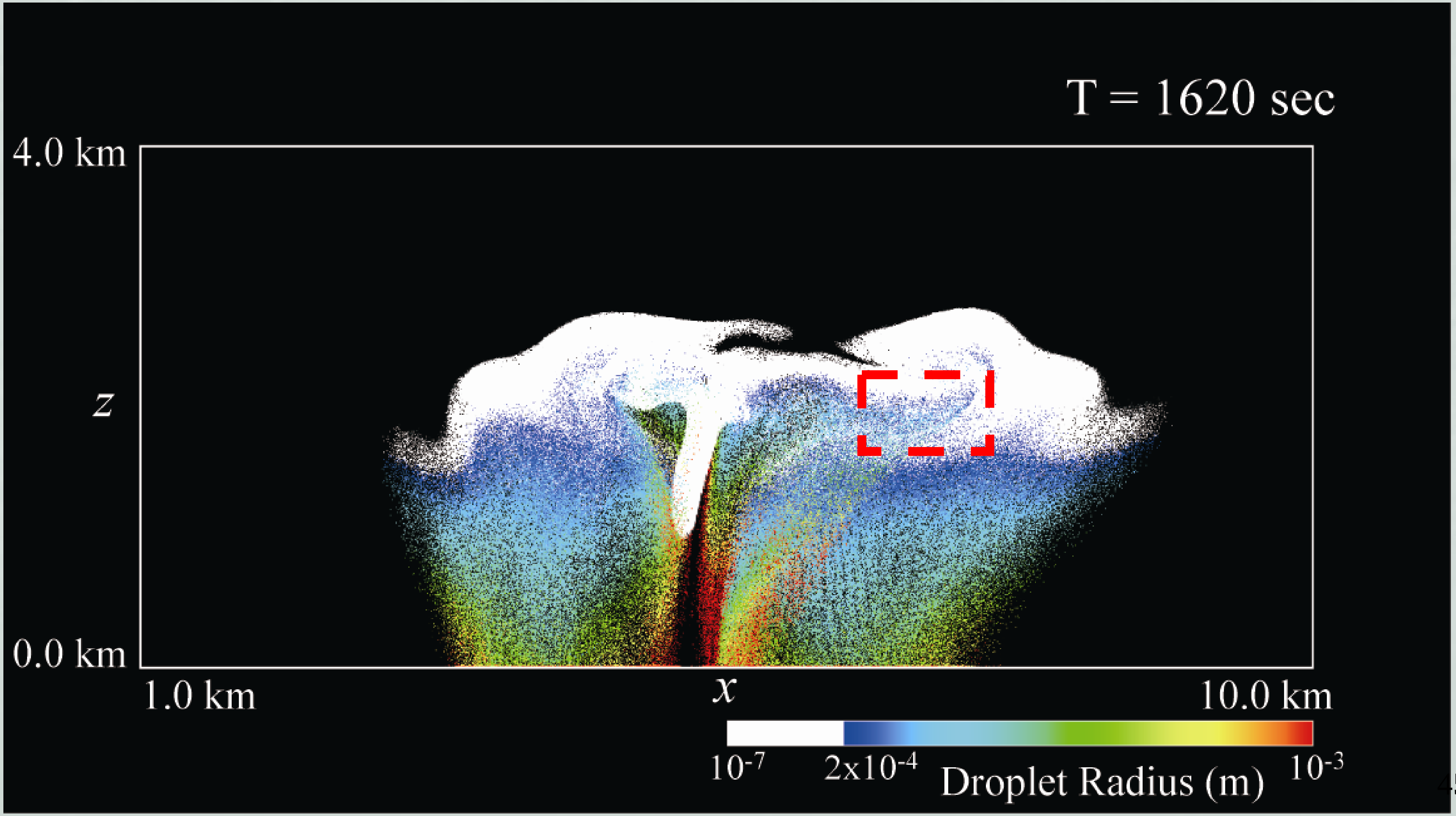
In S.S. et al (2009) we employed "constant multiplicity" method.

This is not be recommended. (Unterstrasser et al. 2017; Dziekan and Pawlowska 2017)

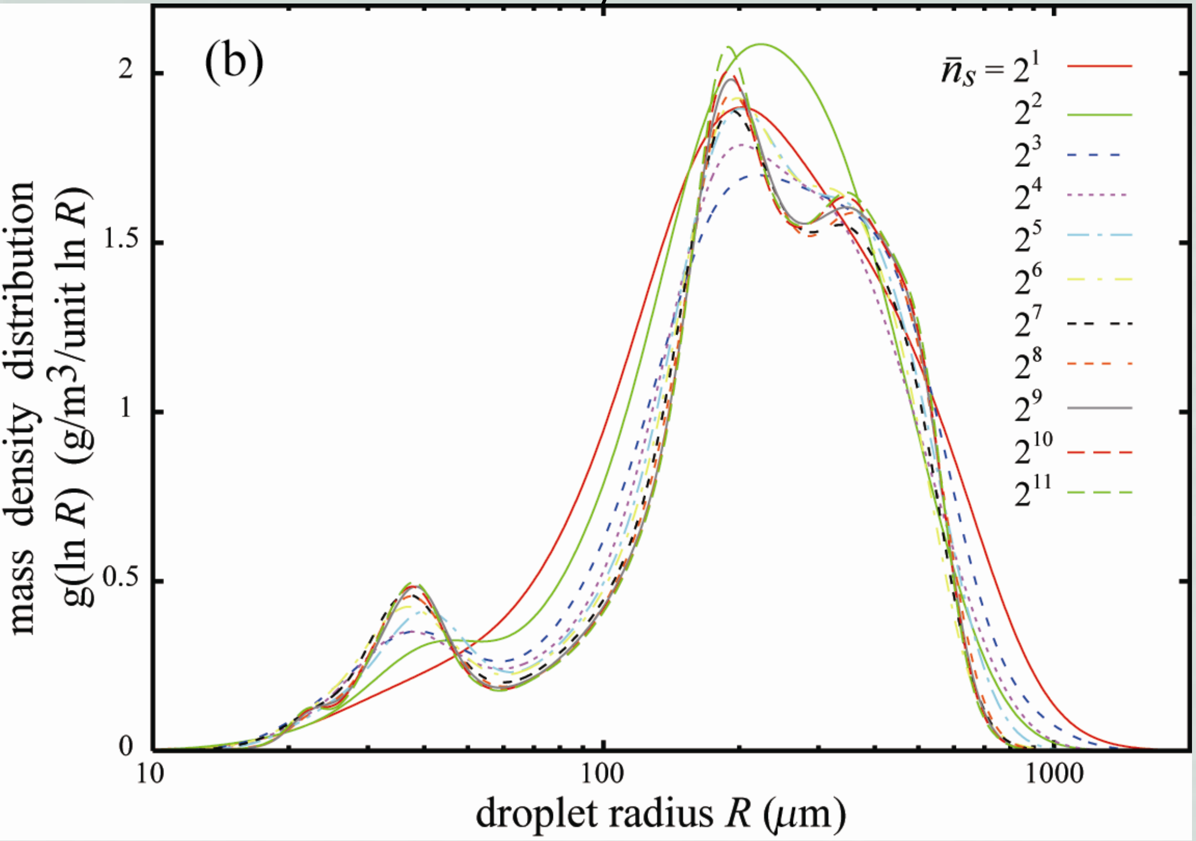
5.3. Isolated Shallow Cumulus (2D, 30min)

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

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



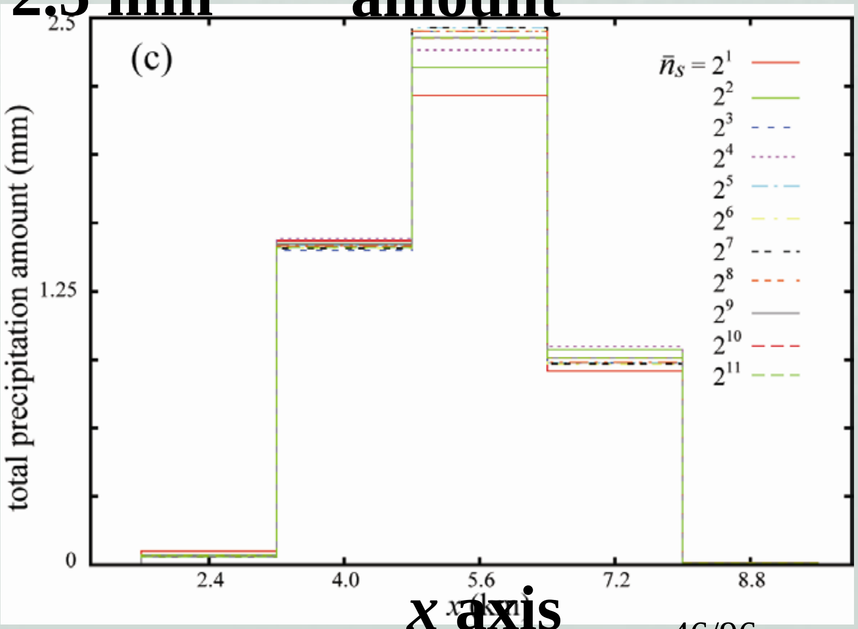
mass density distribution



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

accumulated precipitation amount

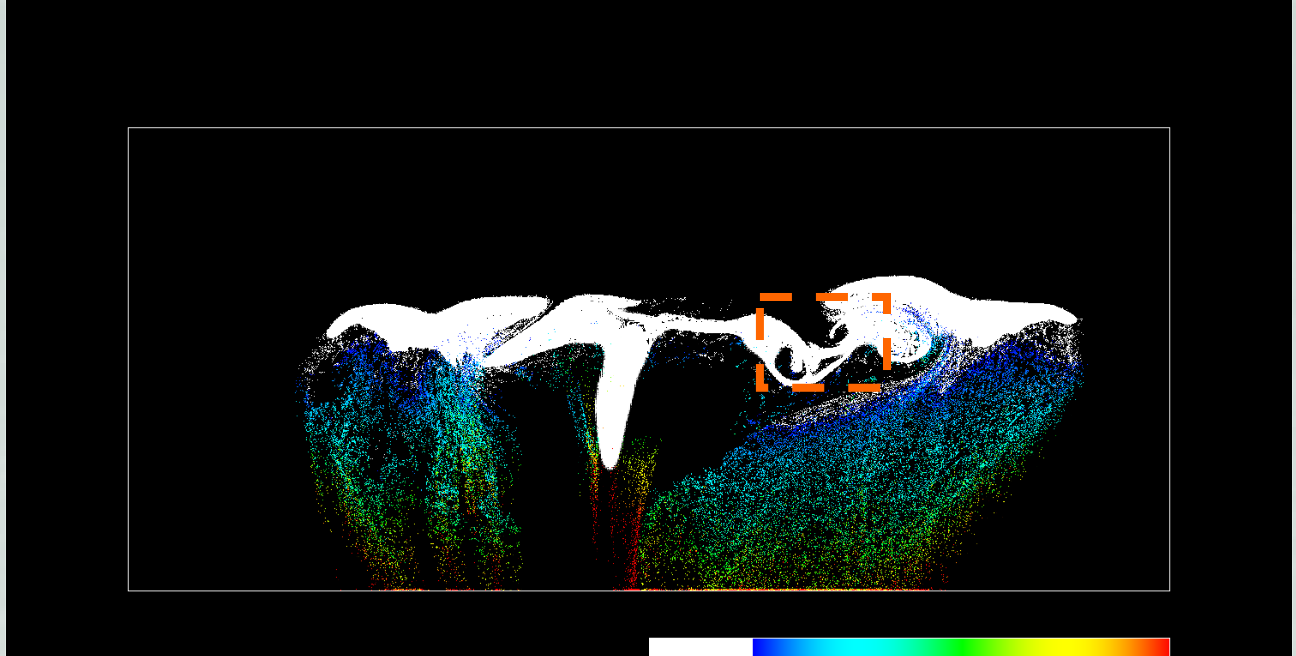
2.5 mm

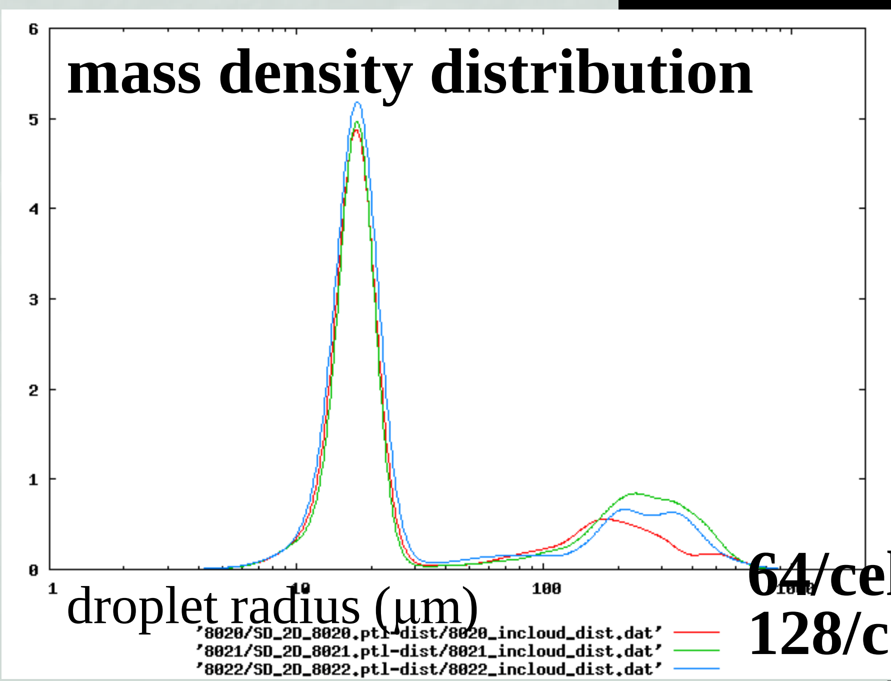


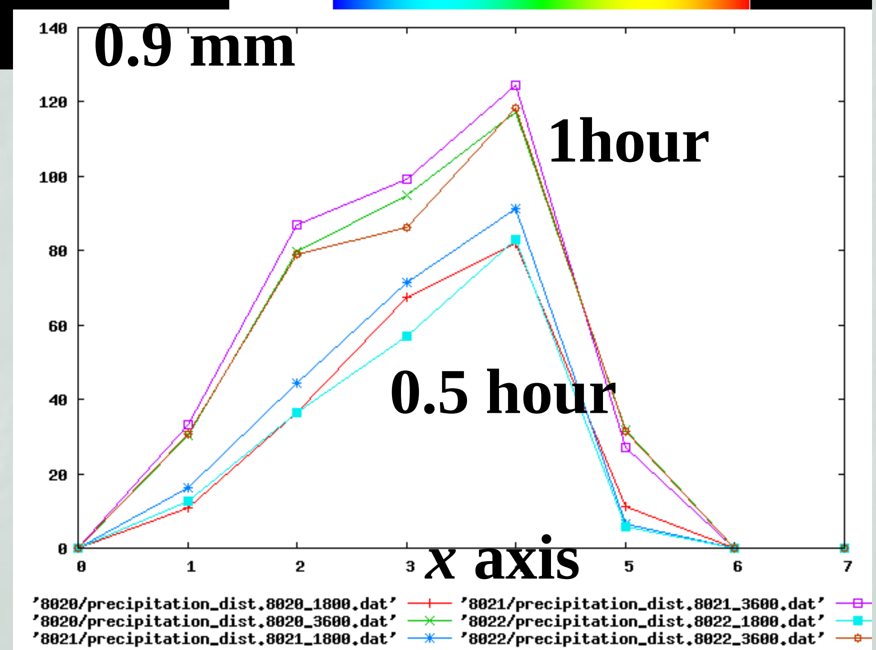
***x* axis**

Good numerical convergence at SDs #32/cell

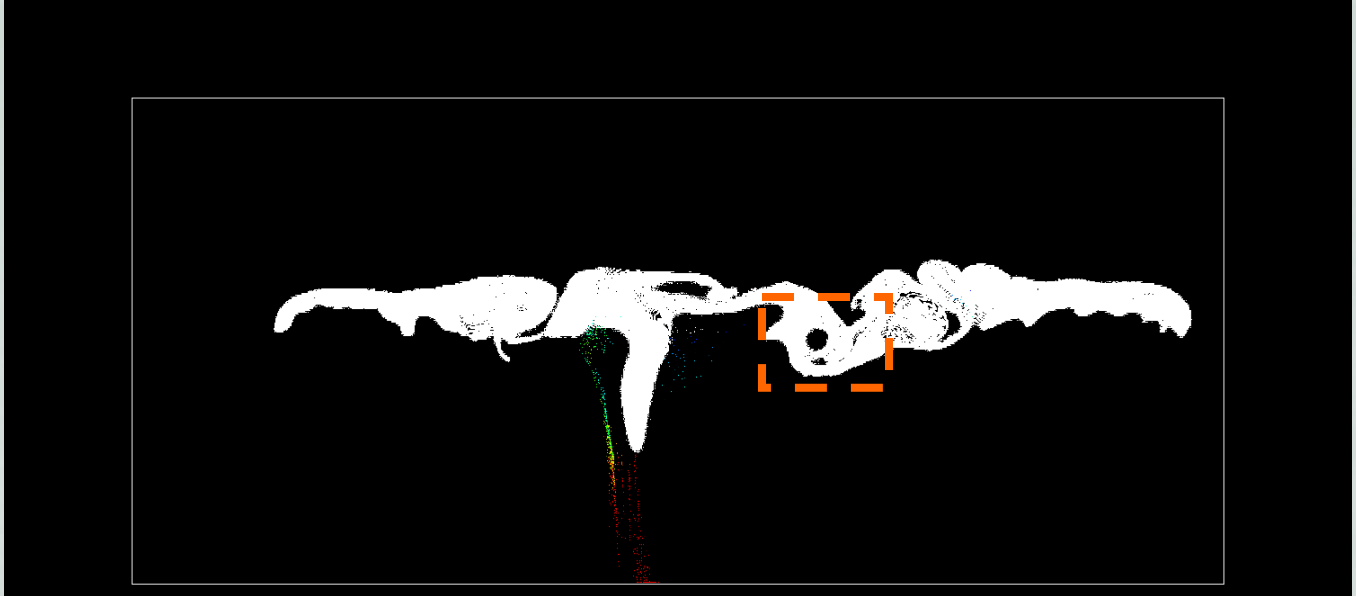
Initially clean case
NaCl aerosol
n=10^8/m^3

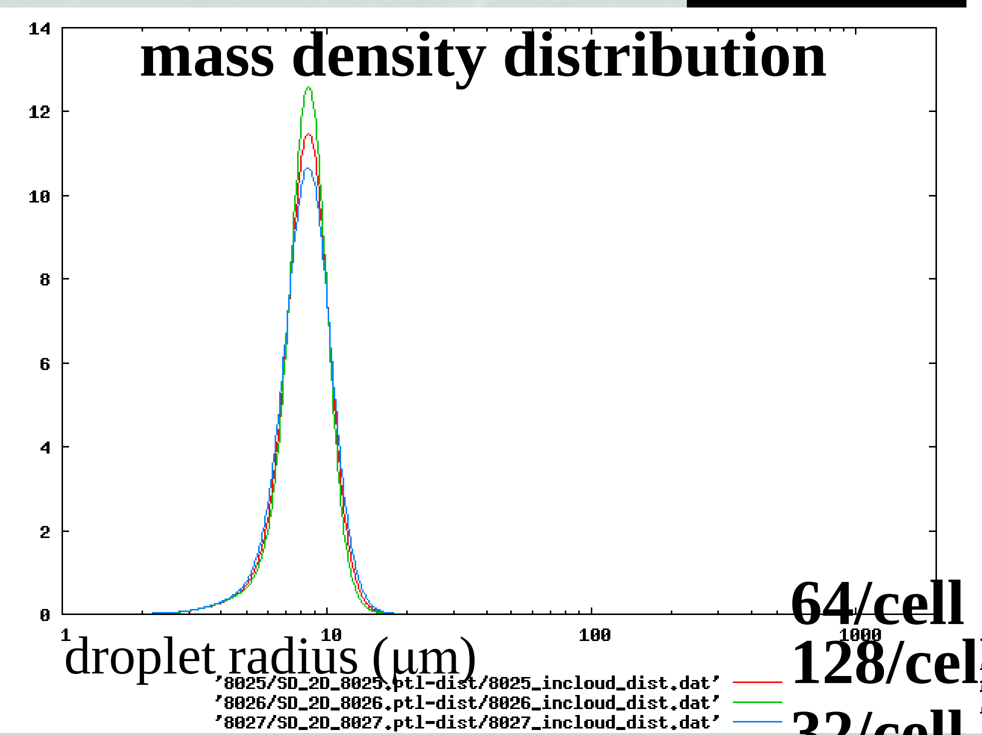


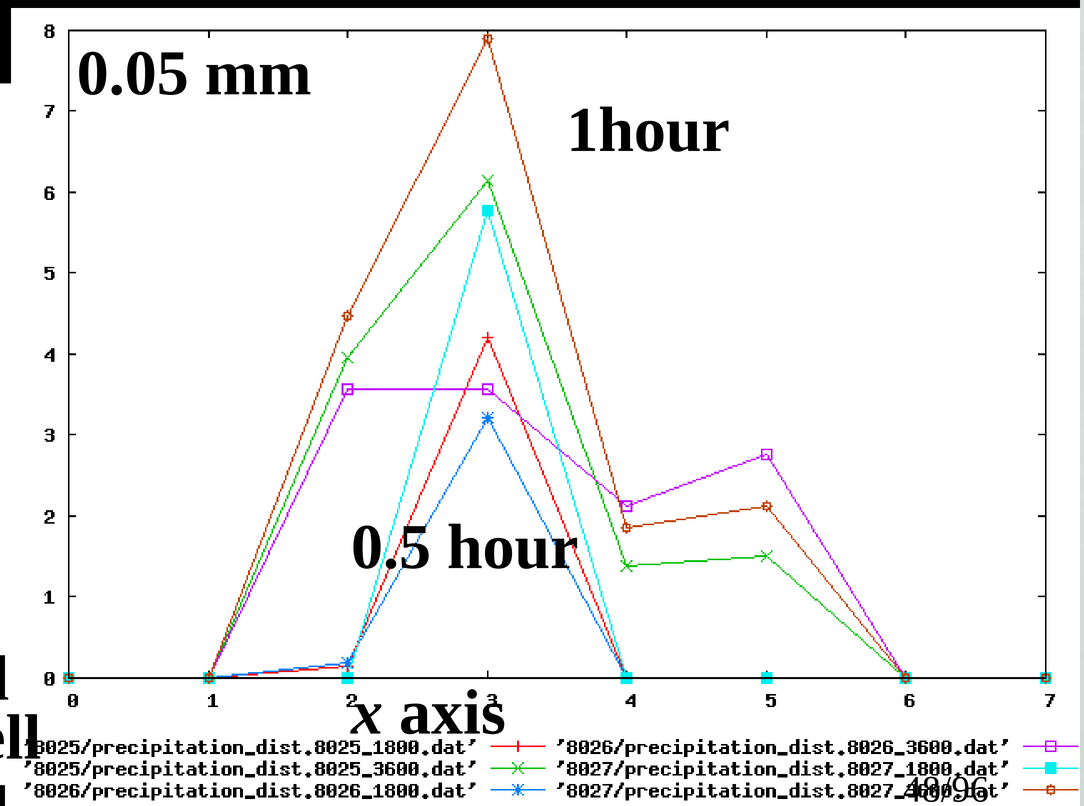




Initially polluted case
NaCl aerosol
n=10^9/m^3



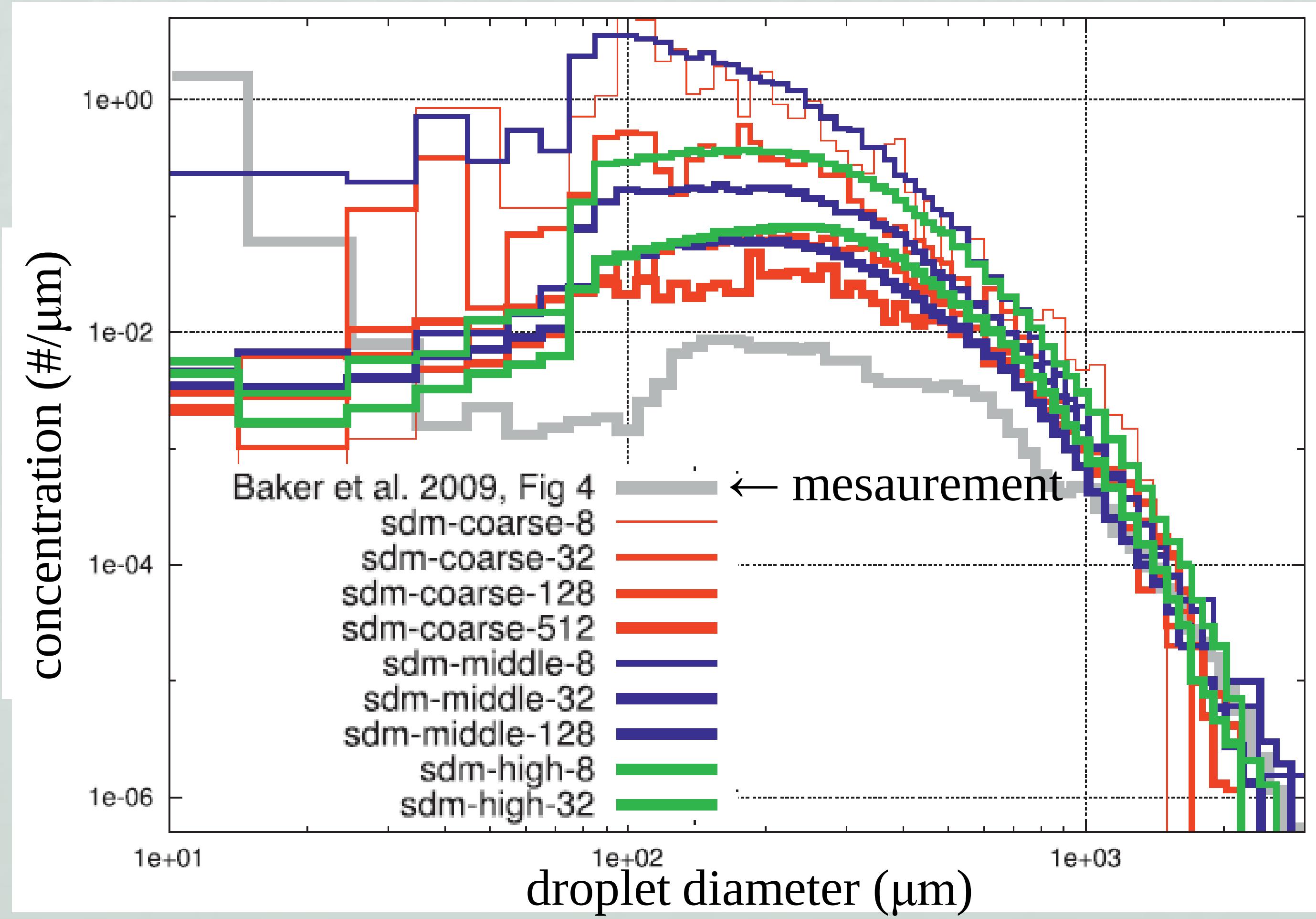




5.4. Shallow Trade Wind Cumuli Field (3D, 24h)

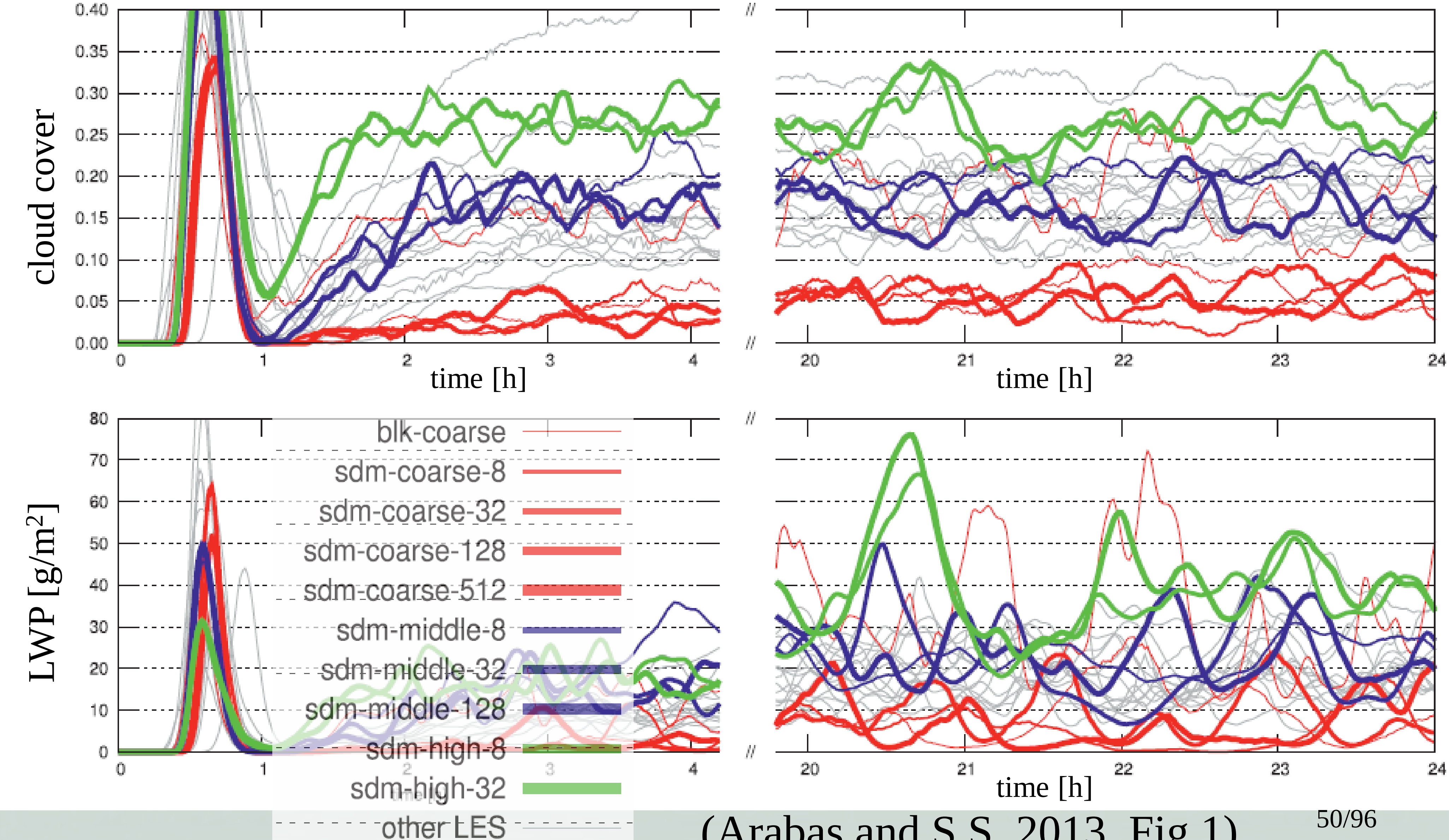
Simulation of precipitating cumuli field is performed based on RICO setup (Arabas and Shima, 2011)

Rain droplet size distribution below cloud based



…cont. (RICO simulation using the SDM)

SDM: (Δx=Δy,Δz) = (100m,40m), (50m,20m), (25m,10m).



(Arabas and S.S. 2013, Fig.1)

Summary of the computational cost of SDM

- 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,
  - To produce a quantitative results, SDs at least #64/cell to at most #8000/cell is needed

6. Advantages of SDM

(Recap) Mesoscopic governing equation of the cloud microphysics

Dynamics of particles with stochastic coalescence

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

$$P_{jk} = K(\boldsymbol{a}_j, \boldsymbol{a}_k)\Delta t / \Delta V.$$

Smoluchowski eq. (for number density of particles)

under decoupling assumption ⇨

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

Here, $n(\boldsymbol{a},\boldsymbol{x},t)$ 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)
  - (Fluid dynamics limit of the Smoluchowski eq.)
- Less accurate
- Very low cost
- **Deriving a reliable bulk model is mathematically challenging but should be pursued**

Spectral (Bin) method (Grabowski et al. (submitted to BAMS))

Eulerian scheme for Smoluchowski eq. using a regular grid

3 issues of Bin

1. Numerical diffusion (Morrison et al. 2018)

   No numerical diffusion in SDM

2. Curse of dimensionality

   Estimated that SDM is faster if num of attributes *d* is large (S.S. et al. 2009)

   Li et al. (2017) confirmed that SDM is indeed faster

3. Breakdown of Smoluchowski eq.

   If the well-mixed volume is small, decoupling cannot be assumed (Alfonso, 2015)

   SDM does not assume decoupling.

   $\xi \to 1$ is a exact limit. (SD→RD)

   Dziekan and Pawlowska (2017) confirmed SDM works even when decoupling is not valid

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?

Lagrangian Particle based Method

- Deterministic: e.g., Andrejczuk et al. 2010; Riechelmann et al. 2012.
  - **Unterstrasser et al. (2017) elucidated that probabilistic method is more efficient**
- Probabilistic: e.g.,
  - SDM (S.S. et al. 2009)
  - O'Rourke (1981): for spray combustion
  - No-Time Counter (NTC) for Smoluchowski eq. (Schmidt and Rutland 2000): for spray combustion
  - DeVille et al. 2011 (Weighted Flow Algorithm): for aerosol dynamics. Implemented on PartMC (Riemer and West)
  - **SDM faster than NTC and O'Rourke (in preparation)**
- WFA vs. SDM is remaining
- Some more schemes in astrophysics area?

6.1. SDM vs. NTC and O'Rourke method

Characteristics

O'Rourke scheme (O'Rourke 1981):

Check all SD pairs ${}_{N}C_{2}$. Cost $O(N^2)$

NTC(No-Time Counter) (Schmidt and Rutland 2000):

Check ${}_{N}C_{2} \cdot P^{(s)}_{\mathrm{max}}$ pairs. Cost $O(N)$

Does not allow multiple coalescence. Accurate but costly

Parallelization is not easy

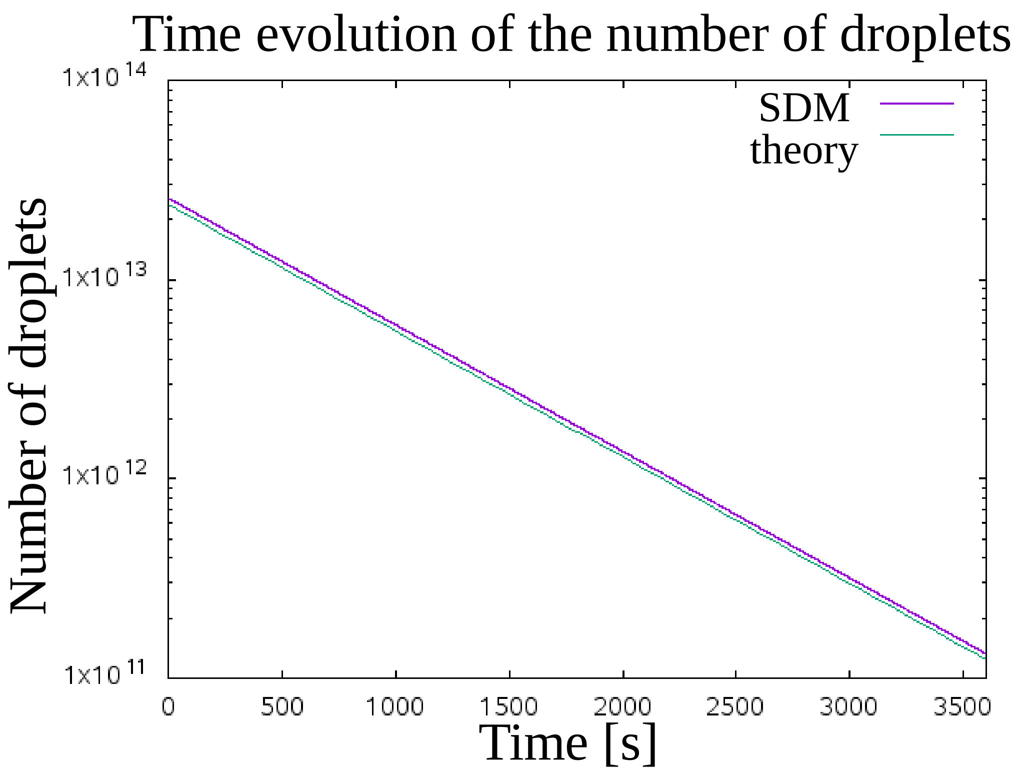
SDM (Super-Droplet Method) (S.S. et al. 2009):

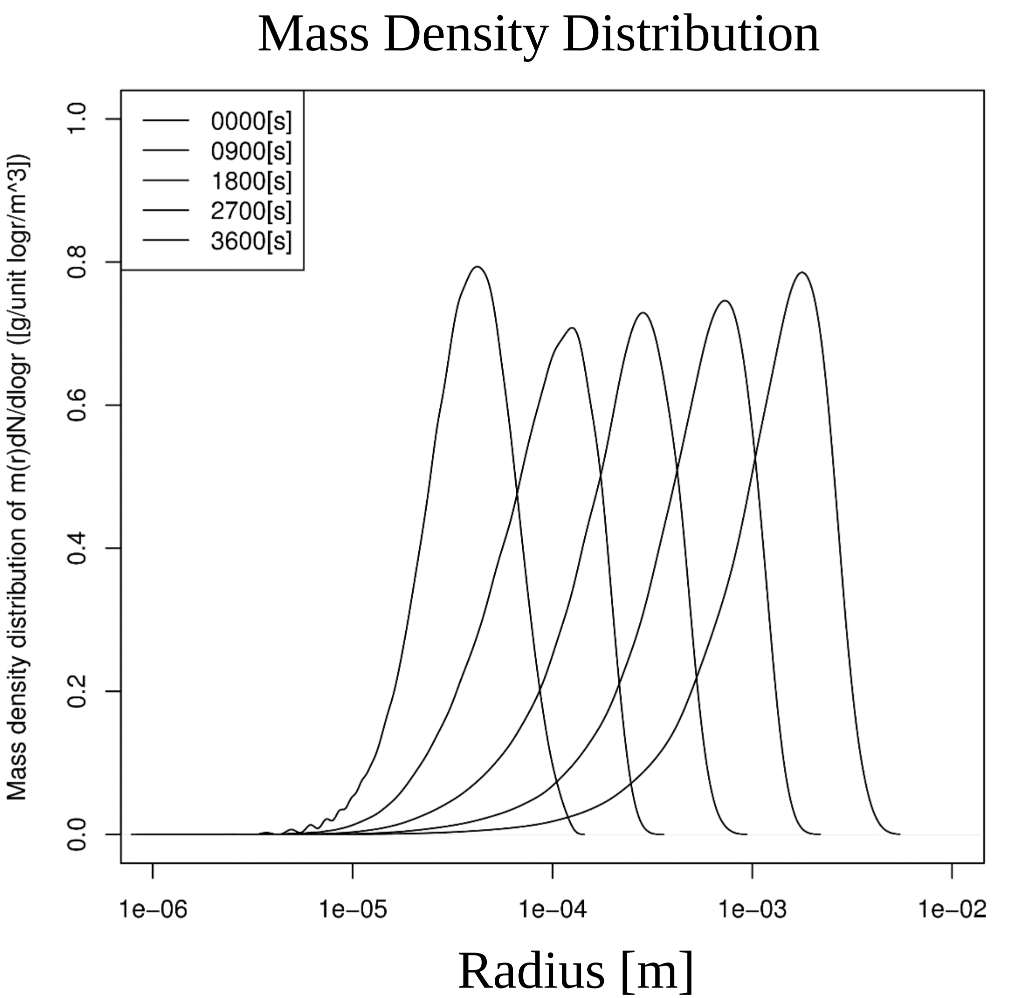
Check $[N/2]$ pairs. Cost $O(N)$

Allow multiple coalescence to reduce the cost.

Parallelization is easy. (No dependence between pairs)

Test with Golovin kernel





Comparison (SDM is way faster)

SDM

Time [s]		SD num											
		80			800			8000			80000		
		all	spray	IO	all	spray	IO	all	spray	IO	all	spray	IO
dt [s]	10	2	0	2	3	1	1	13	6	6	104	60	37
	1	21	0	8	28	9	10	77	35	24	884	546	291
	0.1	193	8	71	276	62	99	759	382	220	8508	5284	2770

NTC

Time [s]		parcel num											
		80			800			8000			80000		
		all	spray	IO	all	spray	IO	all	spray	IO	all	spray	IO
dt [s]	10	4	0	1	11	9	0	669	668	1	143512	143474	31
	1	20	0	6	84	59	10	4529	4479	30	-		
	0.1	196	7	81	367	140	103	41384	41004	217	-		

O'Rourke collision

Time [s]		parcel num											
		80			800			8000			80000		
		all	spray	IO	all	spray	IO	all	spray	IO	all	spray	IO
dt [s]	10	4	0	4	13	11	1	955	949	2	more than 38h		
	1	23	1	12	126	104	8	9524	9472	30	-		
	0.1	207	19	63	1242	1025	87	94985	94538	242	-		

7. Various Applications of the SDM

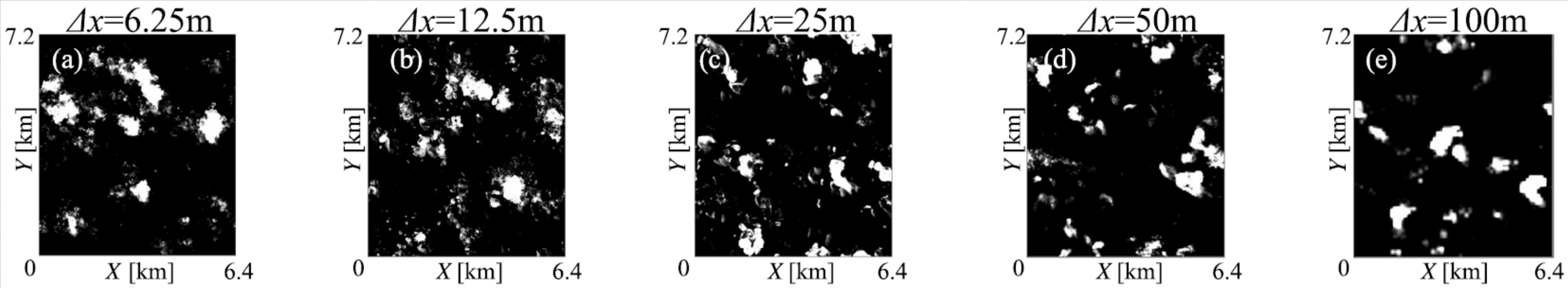
Warm clouds

Shallow cumulus (e.g., Arabas and Shima 2013 (RICO); Sato, Shima, and Tomita 2017, 2018 (BOMEX))

Comparison to observations, and bulk model

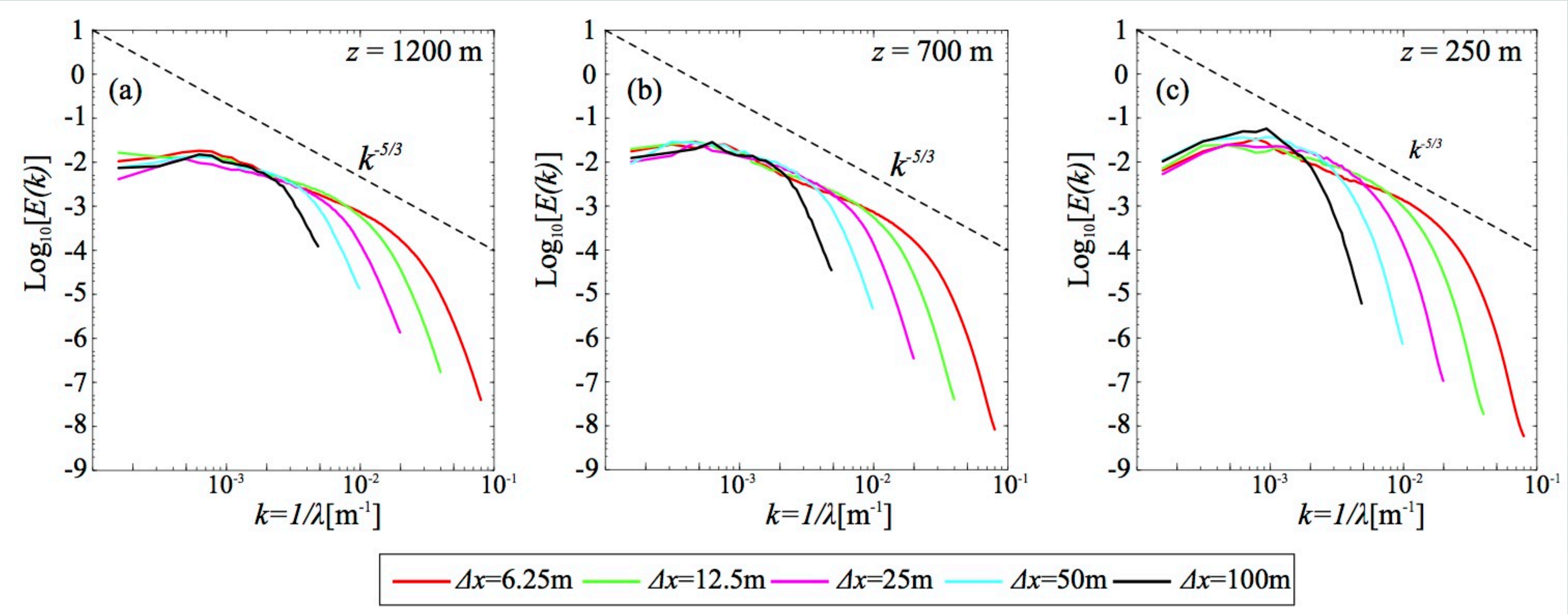
Check the numerical convergence (SD num, grid, *dt*)

Time evolution of cloud pattern (LWP[g/m^2])



$\Delta x = \Delta y = 1.25 \Delta z$ (Sato et al. 2018, Fig.6)

(Flatter turbulence kinetic energy spectrum)



(Sato et al. 2017, Fig.4)

The spectrum in cloud layer is flatter than −5/3 power law

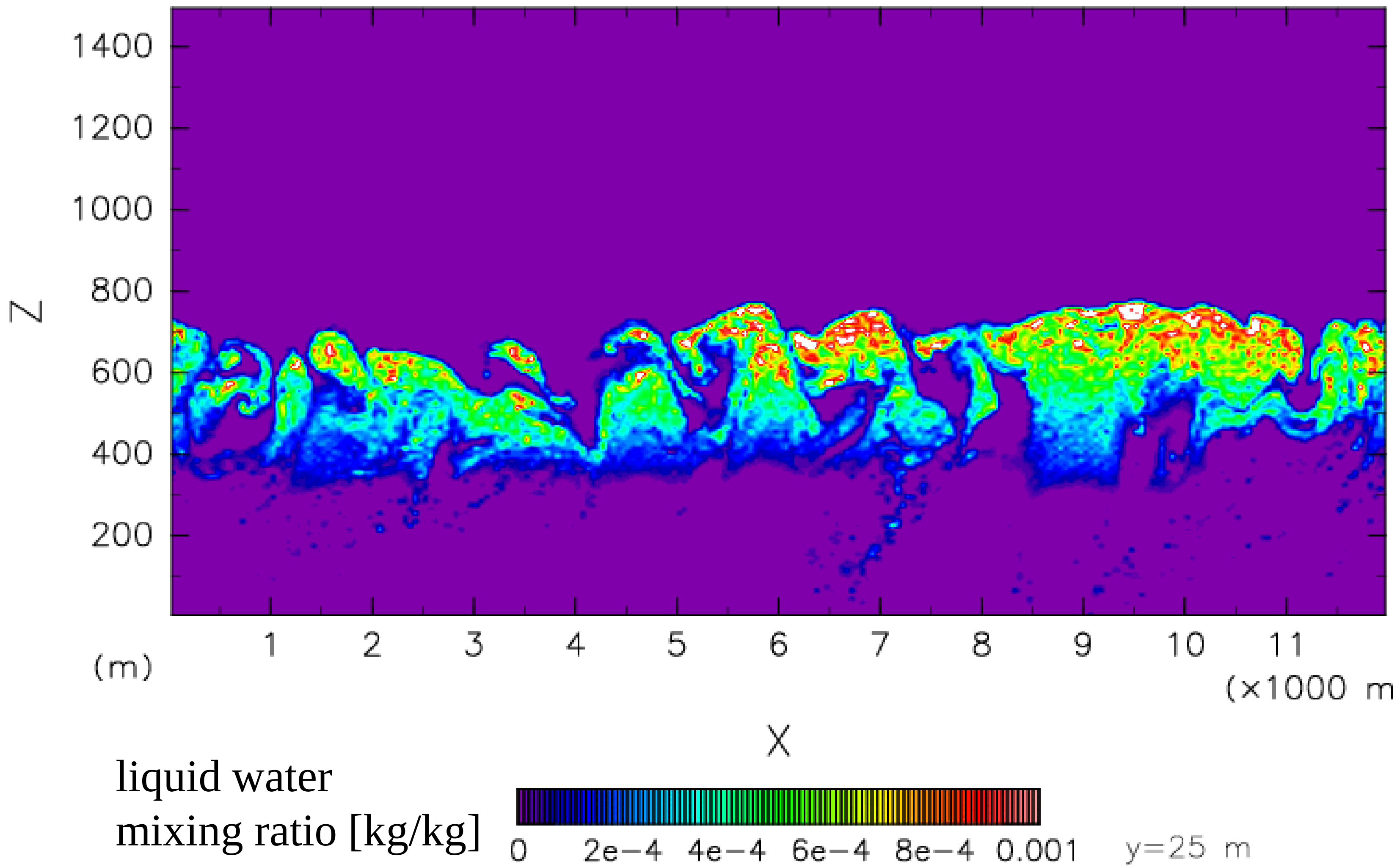
Various size cumuli produce and dissipate energy at various scales?

Not consistent with measurement? (Siebert et al. 2006)

Stratocumulus

2D simulation based on DYCOMS-II RF02 setup (Ackerman et al. 2009)

Proceed to 3D. Can be applied also to fog.



liquid water mixing ratio [kg/kg]

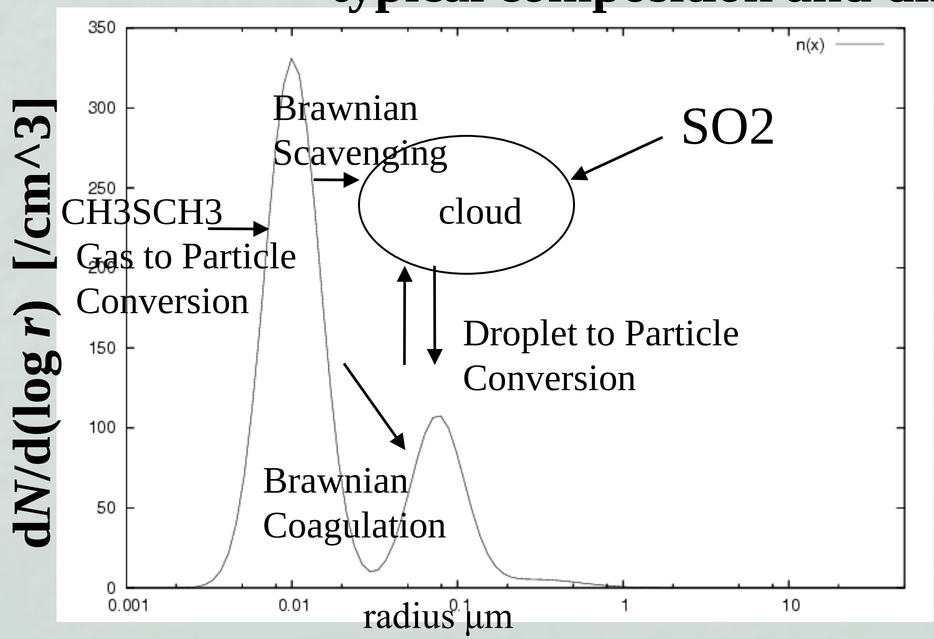
Aerosol processing and aqueous/surface chemistry

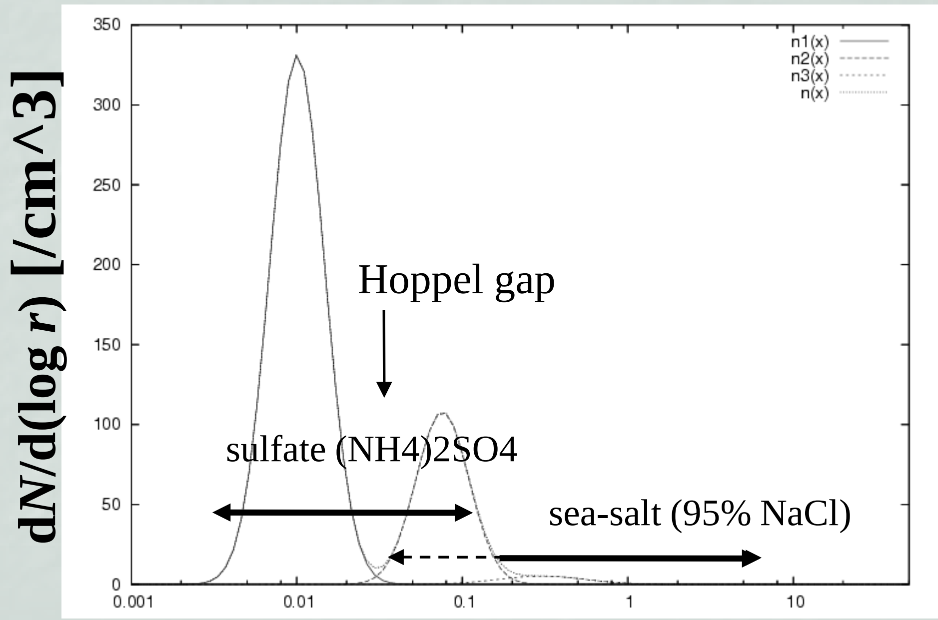
Indispensable when discussing cloud-aerosol **interaction**

We can incorporate it directly using SDM

Jaruga and Pawlowska (2018) reproduced the formation of Hoppel gap from the first princple

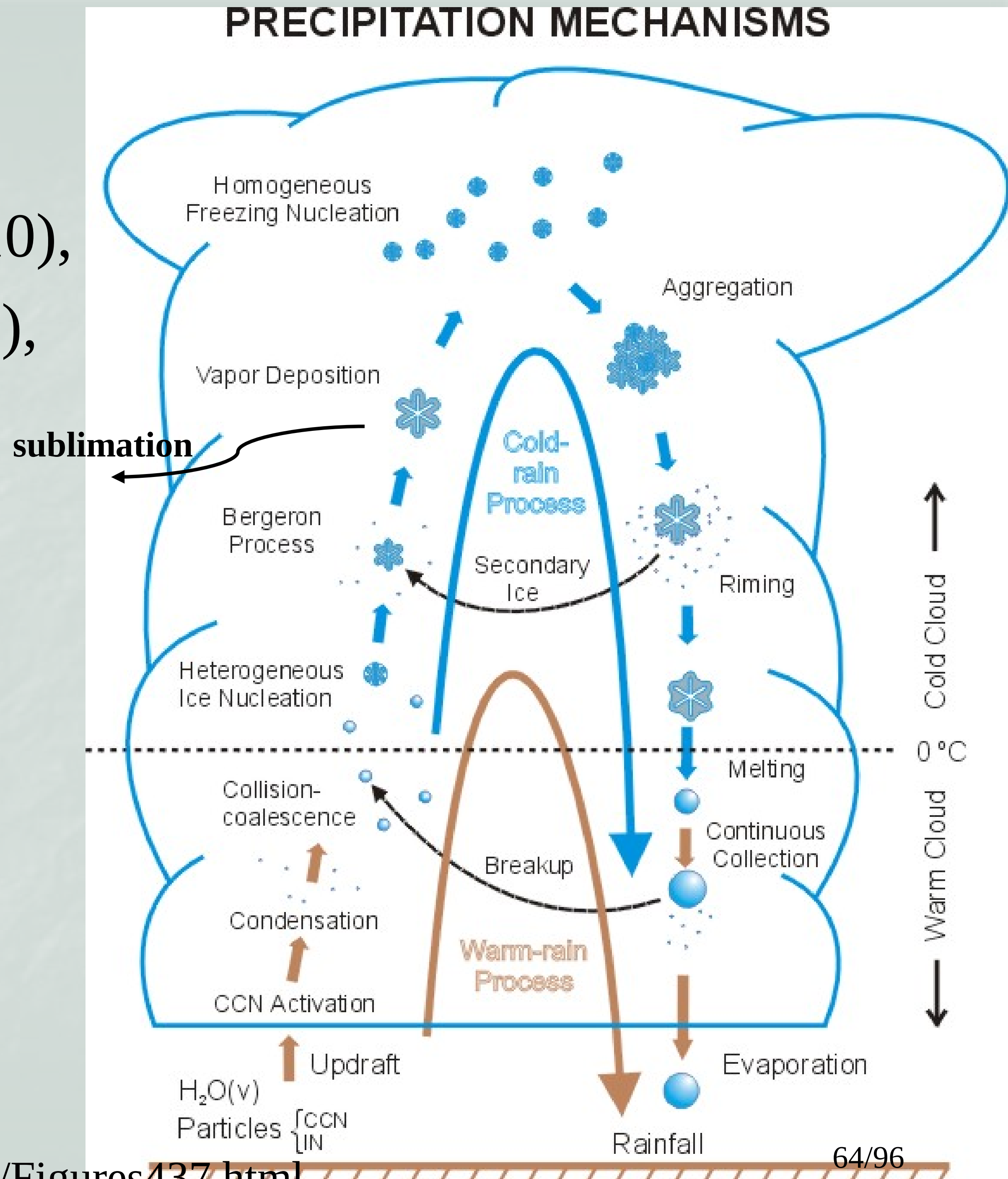
typical composition and distribution of maritime aerosols





Mixed-phase Clouds
(Ice and Liquid water)

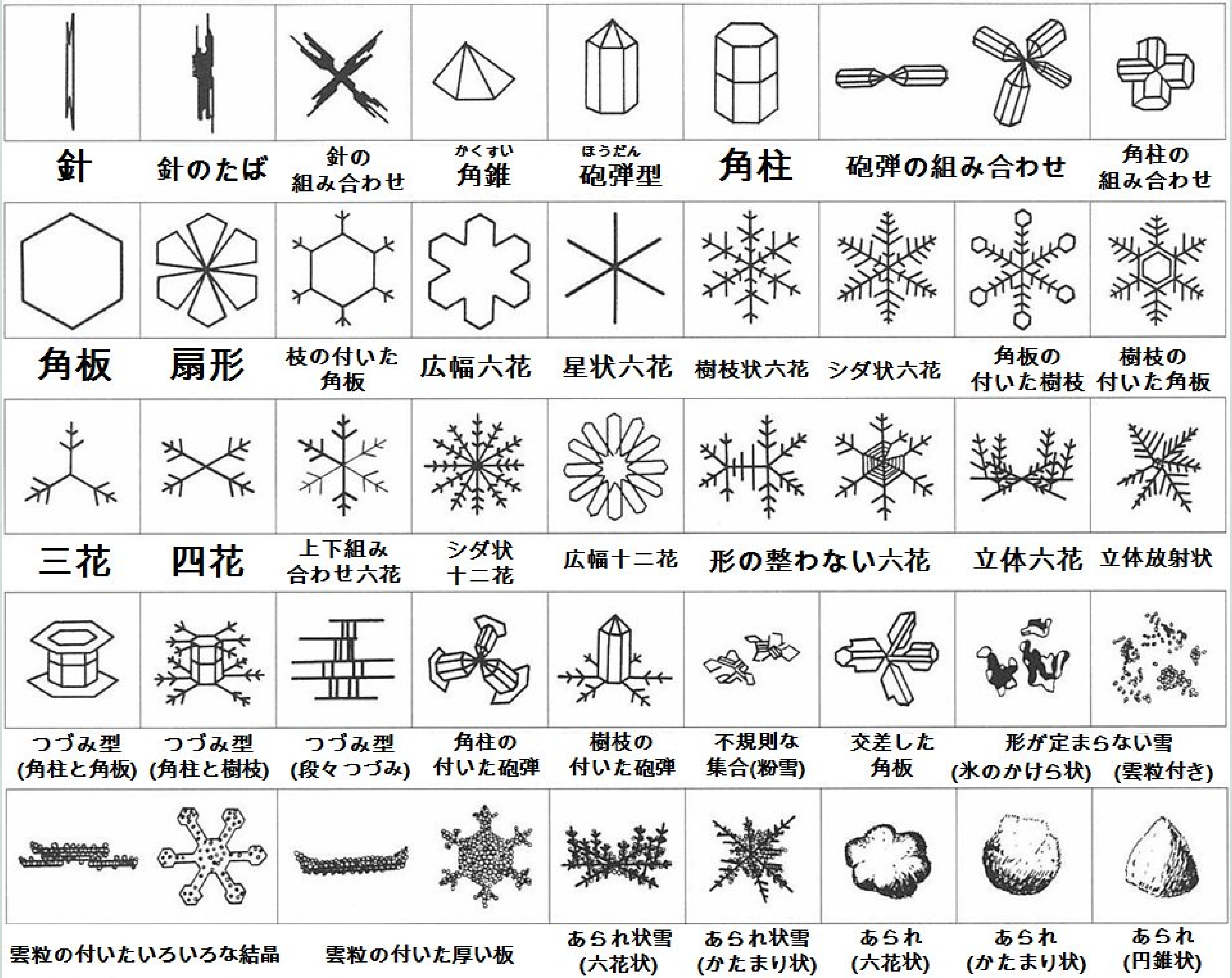
Sölch and Kärcher (2010),
Brdar and Seifert (2018),
Shima et al. (to be
submitted to GMDD)



From "Precipitation Mechanisms" in
http://www.ems.psu.edu/~lno/Meteo437/Figures437.html

Various morphology of ice particles

http://www.mri-jma.go.jp/Dep/fo/fo3/araki/snowcrystals.html#sample



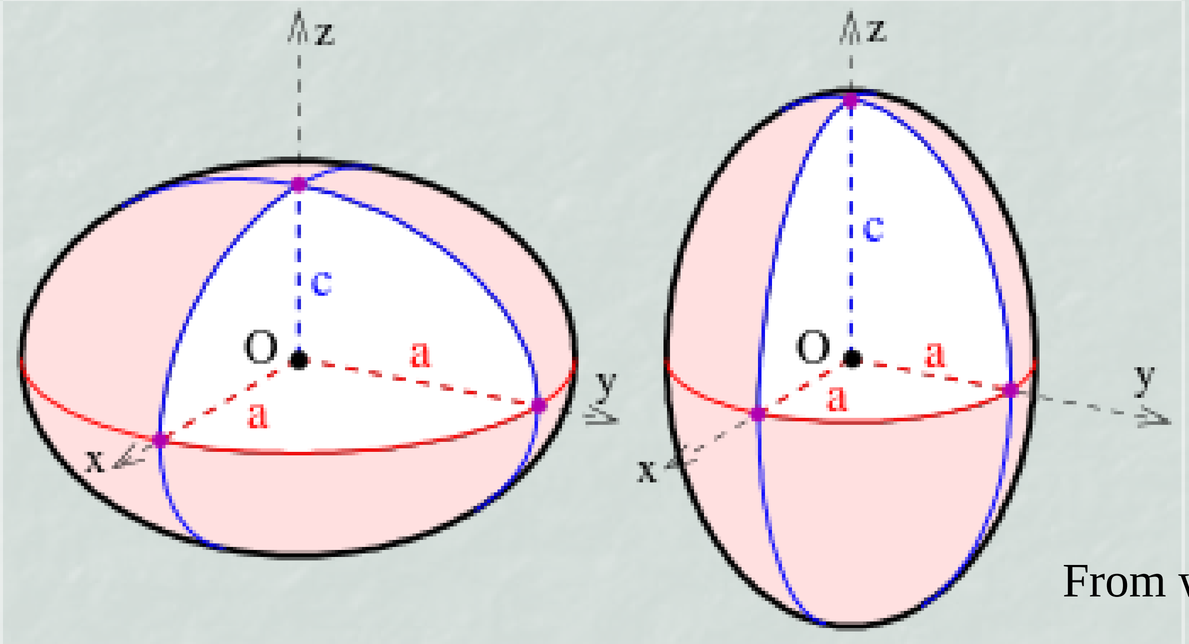
中谷宇吉郎『Snow Crystals』(1954)による

photo by K. Araki

Araki (2014)「雲の中では何が起こっているのか」

Following the idea of the multicomponent bin model (Chen and Lamb 1994, Misumi et al. 2010, Jensen and Harrington 2015)

Ice particles are represented by porous spheroids



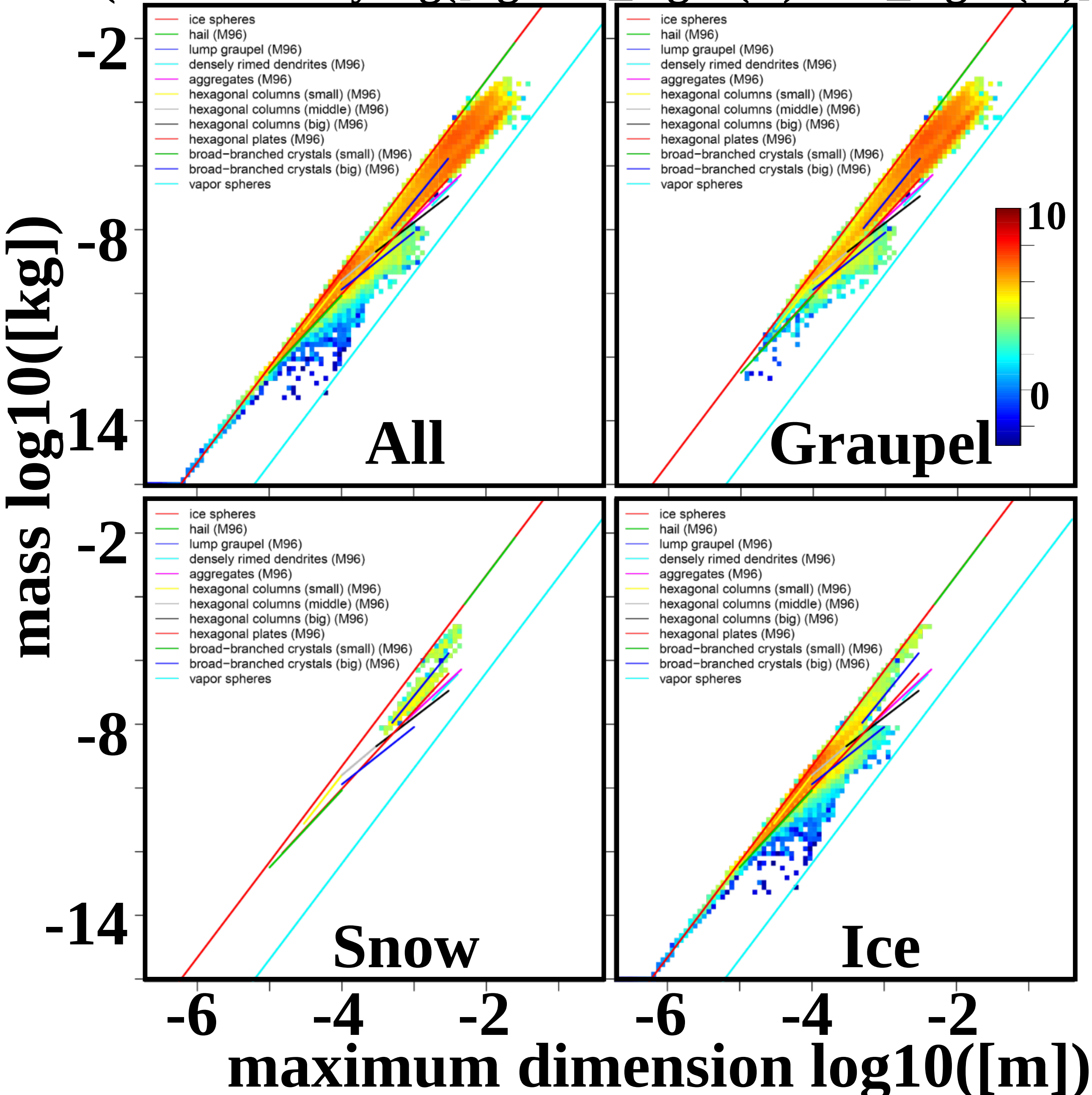
From wikipedia

IN: Freezing temperature strategy

Can account for homogeneous/condensation/immersion freezing

Mass−Dimension

(Mass Density log([kg/unit_log10(*D*)/unit_log10(*m*)]))



More result of cumulonimbus simulation is available from

https://ams.confex.com/ams/15CLOUD15ATRAD/webprogram/Handout/Paper346467/poster076.Shima.pdf

SGS turbulence modeling

- Turbulence affects cloud microphysics in various ways
- Influence onto collision-coalesce can be incorporated by modifying the kernel. (e.g., Wang et al. 2008, Onishi et al. 2015, Chen et al. 2018)
- **Supersaturation and velocity fluctuation through eddy-hopping and entrainment can be incorporated using the SDM**
  - By adding 4 new attributes (S’,U’,V’,W’) (Grabowski and Abade 2017, Abade et al. 2018)
  - By introducing Linear Eddy Model (Hoffman et al., under review)

8. Towards Further Acceleration

- SDM is computationally demanding
- Can we simulate much faster? without losing accuracy??
  - Use SDM **only for rain droplets** (Naumann and Seifert 2015)
  - Twomey SDM: use SDM **only for cloud/rain droplets** (Grabowski et al. 2018)
  - Derive reliable bulk model from Smoluchowski eq.?
    - Not like Boltzmann eq., no stable equilibrium solution
    - But self-similar solutions exists for some kernels (Menon and Pego, 2004)
    - **Regarding those self-similar solutions as the reference, maybe we can derive a bulk model through perturbation expansion or renormalization**

9. Code Availability

Dr. Sylwester Arabas made a comprehensive list

See p.11 of http://slayoo.home.staszic.waw.pl/talk-houghton-20180719.pdf

recent research software (re)developments:

- INC/LCM from LLNL/Leeds,
- EULAG-LCM (`http://www.mmm.ucar.edu/eulag/`) from NCAR/DLR,
- PALM-LES (`http://palm.muk.uni-hannover.de/`) from Univ. Hannover,
- CReSS (`http://www.rain.hyarc.nagoya-u.ac.jp/`) from Univ. Nagoya,
- UCLA-LES (`http://github.com/uclales`) from UCLA/MPI-M,
- Pencil-Code (`http://pencil-code.nordita.org`) from Nordita/UC,
- SCALE (`http://scale.aics.riken.jp/`) from RIKEN,
- UWLCM (`http://github.com/igfuw/UWLCM`) from Univ. Warsaw,
- ICON/McSnow (`http://gitlab.com/sbrdar/mcsnow`) from DWD.

10. Summary

- Super-Droplet Method (SDM) is a particle-based scheme to simulate cloud-microphysics accurately. (S.S. et al. 2009)
- Basic framework and its advantages were presented
  - Should be accurate and faster than bin schemes
- Various applications
  - Warm clouds
  - Aerosol processing and aqueous/surface chemistry
  - Mixed-phase clouds (ice and liquid water)
  - SGS turbulence modeling
- Possibility of further acceleration
  - Twomey SDM
- Showed a list of various available codes

Thank you for your attention!

Acknowledgement

Computers and Funds

This research used computational resources of the K computer and FX10 of the HPCI system provided by the RIKEN AICS and Kyushu University through the HPCI System Research Project (Project ID: hp140094, 150153). ES provided by JAMSTEC was also used.

This research is supported by JSPS KAKENHI Grant-in-Aid for Scientific Research(B): (26286089). and by the JSPS Grant-in-Aid for Young Scientists (B) (15K17756).

This research was supported by the Center for Cooperative Work on Computational Science, University of Hyogo. Y.S is supported by RIKEN special postdoctoral researcher program.

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