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

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

Cloud Dynamics
- Dry air, vapor, trace gas.
- Nucleation from gases or rolling up of dusts

Cloud Microphysics
- Particles (aerosol/cloud/precipitation)
- Chemical reactions
- Condensation precipitation
- Coalescence
- 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
- Droplet dynamics with deterministic collision-coalescence
  - Smoluchowski eq. (Number density dynamics)
    - semi-empirical
    - bulk model (closure in lower moments)
- Droplet dynamics with stochastic collision-coalescence
  - well-mixed ansatz
  - decoupling assumption

Analogy in Fluid Dynamics
- Molecular dynamics with deterministic collision
  - Boltzmann eq. (Number density dynamics)
    - local equilibrium
  - Navier-Stokes eq. (closure in lower moments)
- Molecules dynamics with stochastic collision
  - molecular chaos ansatz
  - decoupling assumption

SDM
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

\( x(t) \): the position of a particle

\( a(t) = \{a^{(1)}(t), a^{(2)}(t), \ldots, a^{(d)}(t)\} \): 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

\[ \{(x_i(t), a_i(t)) | i = 1, 2, \ldots, N_r(t)\} \]
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:

\[
\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{a}_i}{dt} = \mathbf{f}(\mathbf{a}_i), \quad i = 1, 2, \ldots, N_r(t).
\]

Here, \( \mathbf{v}_i \) is the velocity of the particle.

\( \mathbf{v}_i \) is regarded as one of the attribute variables

In general, \( \mathbf{f} \) 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. All the pair $(j, k)$ inside $\Delta V$ have some possibility to coalesce.

$$P_{jk} = C(a_j, a_k) |v_j - v_k| \frac{\Delta t}{\Delta V}$$

$$= K(a_j, a_k) \frac{\Delta t}{\Delta V}$$

= probability that droplet $j$ and $k$ inside a small region $\Delta V$ will coalesce in a short time interval $(t, t + \Delta t)$.

All the pair $(j,k)$ inside $\Delta V$ have some possibility to coalesce.

In general $C$ and $K$ also depend on fluid field.
These are the mesoscopic basic equations of cloud microphysics. Another mesoscopic representation follows.

**Smoluchowski eq. (Stochastic Coalescence Equation; SCE)**

Let \( n(a, x, t) \) be the number density of particles at time \( t \), at \( x \), with attribute \( a \). **Under the decoupling assumption** \( p(n_1, a_1, n_2, a_2) = p(n_1, a_1)p(n_2, a_2) \) etc., we can derive

\[
\frac{\partial n(a, x, t)}{\partial t} + \nabla_x \cdot \{vn\} + \nabla_a \cdot \{fn\} = \frac{1}{2} \int d^d a' n(a') n(a'') K(a', a'') \\
- n(a) \int d^d a' n(a') K(a, a').
\]

Here, \( a' \rightarrow a'' = a \). **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

\[ \{(x_i(t), a_i(t)) | i = 1, 2, \ldots, N_r(t)\} \]

\(x(t)\): the position of the particle

State of a particle is described by 5 attribute variables:

\(a(t) = \{\text{velocity } v, \text{ equivalent radius of water } R, \text{ mass of ammonium sulfate } M\} \)

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

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

If particles are always moving with the terminal velocity,

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

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

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

Beard’s formula (1976) is famous

Terminal velocity suddenly increases when it’s larger than 100μm $\rightarrow$ 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

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

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

\[
F_k(T_i^*) = \left( \frac{L}{R_v T_i^*} - 1 \right) \frac{L \rho_{\text{liq}}}{K T_i^*},
\]

\[
F_d(T_i^*) = \frac{\rho_{\text{liq}} R_v T_i^*}{D e_s(T_i^*)}.
\]
…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 $10^{-16} \text{g}$ at $293 \text{K}$ 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 \( \Delta V \).

2 particles sweep the volume \( \pi(R_j+R_k)^2 |\mathbf{v}_j-\mathbf{v}_k| \Delta t \)

during a small time interval \((t, t+\Delta t)\).

If \( \Delta V \) 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 \( \Delta V \):

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

However,
...cont. (Coalescence of particles by the gravitational settling)

this evaluation is not good for small droplets

Small droplet could swept aside, or bounce

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

\[
P_{jk} = E(R_j, R_k) \pi (R_j + R_k)^2 |v_j - v_k| \frac{\Delta t}{\Delta V}.
\]

e.g., theories of Davis(1972), Jonas(1972), Hall(1980)
Contour plot of $P_{jk}$ as a function of $R_j$ and $R_k$
$\Delta V=1\text{cm}^3$, $\Delta t=1\text{s}$, 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

\[
\rho \frac{D \mathbf{v}}{Dt} = -\nabla P - \rho \mathbf{g} + S_m, \quad \text{motion eq.}
\]

\[
P = \rho R_d T, \quad \text{eq. of state}
\]

\[
\frac{D \theta}{Dt} = -\frac{L}{c_p \Pi} S_v, \quad \text{energy eq.}
\]

\[
\frac{D \rho}{Dt} = -\rho \nabla \cdot \mathbf{v}, \quad \text{continuity eq.}
\]

\[
\frac{D q_v}{Dt} = S_v. \quad \text{mass coupling}
\]

\[
S_m(r,t), \quad S_v(r,t)
\]

Coupling term to microphysics process

density of liquid water / unit space volume

mass of evaporated liquid water/ unit space volume /unit time/ρ
3. Super-Droplet Method

Mesoscopic governing equation of the cloud microphysics

Dynamics of particles with stochastic coalescence

\[
\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{a}_i}{dt} = \mathbf{f}(\mathbf{a}_i), \quad i = 1, 2, \ldots, N_r(t).
\]

\[
P_{jk} = K(\mathbf{a}_j, \mathbf{a}_k) \Delta t / \Delta V.
\]

Smoluchowski eq. (for number density of particles)

under decoupling assumption

\[
\frac{\partial n(\mathbf{a}, \mathbf{x}, t)}{\partial t} + \nabla_x \cdot \{ \mathbf{v} n \} + \nabla_\mathbf{a} \cdot \{ \mathbf{f} n \}
\]

\[
= \frac{1}{2} \int d^d \mathbf{a}' n(\mathbf{a}') n(\mathbf{a}'') K(\mathbf{a}', \mathbf{a}'')
\]

\[- n(\mathbf{a}) \int d^d \mathbf{a}' n(\mathbf{a}') K(\mathbf{a}, \mathbf{a}').
\]

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
Hereafter, 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** $\xi$, position $x$, and attribute $a$

Each SD represents $\xi$ number of real-droplets $(x,a)$

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

$$\{(\xi_i(t), x_i(t), a_i(t))|i = 1, 2, \ldots, N_s(t)\}$$

SD can be regarded as a weighted sample of RDs

Note that $\xi$ is time dependent (Detail follows)
Dynamics of super-droplets

Individual dynamics

Same as real-droplets, they obey

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

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

After the coalescence event, we define that a big SD with $\xi_1$, 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

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

Check) Consider coalescence between $\xi_j$ num of RD $a_j$ and $\xi_k$ num of RD $a_k$. Expected num of coalesced pairs is

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

Coalescence of SDs ($\xi_j, a_j$) and ($\xi_k, a_k$) corresponds to coalescence of $\min(\xi_j, \xi_k)$ pairs of RD $a_j$ and $a_k$

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

$$E_{jk}^{(s)} = \min(\xi_j, \xi_k) P_{jk}^{(s)} \quad \leftarrow \text{Super-Droplet World}$$

$$= \min(\xi_j, \xi_k) \max(\xi_j, \xi_k) P_{jk}$$

$$= \xi_j \xi_k P_{jk}$$

$$= E_{jk}$$
3.2. Numerical Implementation of the SDM

Outlook

Cloud microphysics (= Super-Droplet Method)
Individual dynamics

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

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 $\Delta t$ 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**

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

\[
P = \rho R_d T,
\]

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

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

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

**Numerical scheme**

Evaluate all the terms except *pink terms* with \( \Delta t_f \)

*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.

\[ m_i \frac{d\mathbf{v}_i}{dt} = m_i g + \mathbf{F}_D(\mathbf{v}_i, U(x_i), R_i), \quad \frac{dx_i}{dt} = \mathbf{v}_i, \]

Numerical scheme

\[ \mathbf{v}_i(t) = U_i^* - \hat{z}v_\infty(R_i(t)) \]

\[ x_i(t + \Delta t_m) = x_i(t) + \Delta t_m \mathbf{v}_i(t) \]
Condensation/Evaporation

Basic eqs.

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

\[
F_k = \left( \frac{L}{R_v T} - 1 \right) \frac{L \rho_{\text{liq}}}{K T}, \quad F_d = \frac{\rho_{\text{liq}} R_v T}{D e_s(T)}
\]

\[
S_v(x, t) := \frac{-1}{\rho(x, t)} \sum_{i=1}^{N_r} \frac{d m_i(t)}{d t} \delta^3(x - x_i(t)).
\]

\[
\frac{D \theta}{D t} = -\frac{L}{c_p \pi} S_v + \kappa \nabla^2 \theta,
\]

\[
\frac{D q_v}{D t} = S_v + \kappa \nabla^2 q_v.
\]

Numerical scheme (Implicitly for SDs, explicitly for fluids)

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

\[
S_v(x_{lmn}, t) = \frac{-1}{\rho(x_{lmn}, t)} \sum_{i=1}^{N_s} \xi_i \frac{m_i(t + \Delta t_g) - m_i(t)}{\Delta t_g} w(x_{lmn} - x_i(t)).
\]

(Also update fluid)

\[
\theta(x_{lmn}, t + \Delta t_g) = \theta(x_{lmn}, t) - \Delta t_g \frac{L S_v(x_{lmn}, t)}{c_p \pi(x_{lmn}, t)},
\]

\[
q_v(x_{lmn}, t + \Delta t_g) = q_v(x_{lmn}, t) + \Delta t_g S_v(x_{lmn}, t).
\]
Momentum Transfer from Microphysics

Basic eq.

\[
\rho \frac{DU}{Dt} = -\nabla P - (\rho - \rho_w)g + \lambda \nabla^2 U,
\]

\[
\rho_w(x, t) := \sum_{i=1}^{N_r} m_i(t) \delta^3(x - x_i(t)),
\]

Numerical scheme

\[
\rho_w(x_{lmn}, t) = \sum_{i=1}^{N_s} \xi_i m_i(t) w(x_{lmn} - x_i(t))
\]
Stochastic Coalescence

Basic eq.

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

All the pair \((j,k)\) in \(\Delta V\) have some possibility to coalesce

Translation into a dynamics of SDs

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 \(t + \Delta t_c\)
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) $\rightarrow$ (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

$$p_i := P_{j_ik_i}^{(s)} \frac{N_s'(N_s'-1)}{2} \left[ \frac{N_s'}{2} \right], \quad i = 1, 2, \ldots, \left[ \frac{N_s'}{2} \right].$$

This assures the consistency of expectation value

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

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)

T = 1590 sec
Shallow cumulus (3D, $\Delta z = 8$ m)

grid: 624x1024x1024, particles: #10^{10},
ES 256 nodes
photo realistic visualization:
$\Delta z = 16 \text{ m}$
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 $q(\xi, a; N_s)$

Assuming that

$q(\xi, \bar{a}, t; \alpha N_s) = \alpha^{k_1} q(\alpha^{k_2} \xi, \bar{a}, t; N_s)$

Scaling law of this form exists

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

SDs expected to reproduce RD num density

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

Conservation of $N_s$

$q$ is smooth enough with respect to $\xi$

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

$q(\xi, \bar{a}, t; \alpha N_s) = \alpha^2 q(\alpha \xi, \bar{a}, t; N_s)$
Scaling Relation Between Error and Cost

RD num density \( n(a,t) \) can be estimated from SD population \( \{ (\xi_i, a_i) \mid i=1,\ldots,N_s \} \). Let’s evaluate the error of this.

Applying kernel density estimation (Terrell and Scott 1992),

\[
\tilde{n}(a) := \sum_{i=1}^{N_s} \xi_i W_\sigma^{(d)}(a - a_i).
\]

\[
W_\sigma^{(d)}(a) := \frac{1}{(\sqrt{2\pi}\sigma)^d} \exp \left\{ -\frac{a^2}{2\sigma^2} \right\}.
\]

Evaluate the error by Mean Integrated Squared Error (MISE)

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

Combined with the scaling law of \( q \), we can derive the relation between error \( C(\sigma^*) \) and cost \( N_s \)

\[
\text{operation} \sim N_s \sim \left( \frac{1}{\sqrt{C(\sigma^*)}} \right)^{(d+4)/2},
\]

\[
\text{memory} \sim N_s \sim \left( \frac{1}{\sqrt{C(\sigma^*)}} \right)^{(d+4)/2}.
\]
Computational Cost of Bin method

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

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

Then, we can derive

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

$\text{memory} \sim N_b^d \sim \left( \frac{1}{\sqrt{C}} \right)^{d/k}$

here, $C$ is the error defined by

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

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.
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 \(<r_0> = 30\mu m\))

Much more realistic kernel for simulating clouds

\[ N_s = 2^{13} = 8192 \]

\[ N_s = 2^{17} = 131072 \]

- red line: EFM
- wavy line: SDM

T = 0s
T = 600s
T = 1200s
T = 1800s
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

$$N_s = 2^{13} = 8192$$

$$N_s = 2^{17} = 131072$$
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 $[\log r_{\text{min}}, \log r_{\text{max}}]$ , and assign a multiplicity as follows

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

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

This reduces sampling error and improve the convergence


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/m³)

Particle size distribution in the square region and precipitation amount are investigated for various SD num
initial number density of NaCl aerosol
\( n = 10^7/m^3 \)

accumulated precipitation
2.5 mm amount

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

mass density distribution

droplet radius (μm)

64/cell
128/cell
32/cell

0.05 mm
1 hour

0.5 hour
Simulation of precipitating cumuli field is performed based on RICO setup (Arabas and Shima, 2011)
Rain droplet size distribution below cloud based

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

![Graph showing concentration vs. droplet diameter](image)
…cont. (RICO simulation using the SDM)

SDM: $(\Delta x=\Delta y, \Delta z) = (100\text{m},40\text{m}), (50\text{m},20\text{m}), (25\text{m},10\text{m})$. 

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{\textit{LWP [g/m$^2$]} and \textit{cloud cover} as a function of \textit{time [h]} for different simulations.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure2}
\caption{\textit{LWP [g/m$^2$]} and \textit{cloud cover} as a function of \textit{time [h]} for different simulations.}
\end{figure}

\textit{(Arabas and S.S. 2013, Fig.1)}
Summary of the computational cost of SDM

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

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

\[
\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{a}_i}{dt} = \mathbf{f}(\mathbf{a}_i), \quad i = 1, 2, \ldots, N_r(t).
\]

\[
P_{jk} = K(\mathbf{a}_j, \mathbf{a}_k) \Delta t / \Delta V.
\]

Smoluchowski eq. (for number density of particles)

\[
\frac{\partial n(\mathbf{a}, \mathbf{x}, t)}{\partial t} + \nabla_x \cdot \{\mathbf{v} n\} + \nabla_\mathbf{a} \cdot \{\mathbf{f} n\} = \frac{1}{2} \int d^d \mathbf{a}' n(\mathbf{a}') n(\mathbf{a}'') K(\mathbf{a}', \mathbf{a}'') - n(\mathbf{a}) \int d^d \mathbf{a}' n(\mathbf{a}') K(\mathbf{a}, \mathbf{a}').
\]

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

SDM is not the only way to solve this equation.
Exact Monte Carlo method (Gillespie 1975, Seebelberg 1996)
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.
   $\xi \rightarrow 1$ is a exact limit. (SD $\rightarrow$ 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 \( \binom{N}{2} \). Cost \( O(N^2) \)

NTC (No-Time Counter) (Schmidt and Rutland 2000):
Check \( \binom{N}{2} \cdot P_{\text{max}}^{(s)} \) pairs. Cost \( O(N) \)
Does not allow multiple coalescence. Accurate but costly
Parallelization is not easy

Check \( \lceil N/2 \rceil \) pairs. Cost \( O(N) \)
Allow multiple coalescence to reduce the cost.
Parallelization is easy. (No dependence between pairs)
Test with Golovin kernel

Time evolution of the number of droplets

Number of droplets vs. Time [s]

Mass Density Distribution

Mass density distribution of m(r)dN/dr [g/(unit log/m^3)]

Radius [m]
## Comparison (SDM is way faster)

### SDM

<table>
<thead>
<tr>
<th>Time [s]</th>
<th>80</th>
<th>800</th>
<th>8000</th>
<th>80000</th>
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</thead>
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<tr>
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<td>spray</td>
<td>IO</td>
<td>all</td>
</tr>
<tr>
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<td>2</td>
<td>0</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
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<tr>
<td>0.1</td>
<td>193</td>
<td>8</td>
<td>71</td>
<td>276</td>
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</table>

### NTC

<table>
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<tr>
<th>Time [s]</th>
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<th>800</th>
<th>8000</th>
<th>80000</th>
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<tbody>
<tr>
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<td>spray</td>
<td>IO</td>
<td>all</td>
</tr>
<tr>
<td>10</td>
<td>4</td>
<td>0</td>
<td>1</td>
<td>11</td>
</tr>
<tr>
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<tr>
<td>0.1</td>
<td>196</td>
<td>7</td>
<td>81</td>
<td>367</td>
</tr>
</tbody>
</table>

### O'Rourke collision

<table>
<thead>
<tr>
<th>Time [s]</th>
<th>80</th>
<th>800</th>
<th>8000</th>
<th>80000</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>all</td>
<td>spray</td>
<td>IO</td>
<td>all</td>
</tr>
<tr>
<td>10</td>
<td>4</td>
<td>0</td>
<td>4</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>23</td>
<td>1</td>
<td>12</td>
<td>126</td>
</tr>
<tr>
<td>0.1</td>
<td>207</td>
<td>19</td>
<td>63</td>
<td>1242</td>
</tr>
</tbody>
</table>

- dt [s]: Time [s]
- parcel num: Number of parcels
- SD num: Speed (SDM)
- NTC: Number of tasks completed
- O'Rourke collision: O'Rourke collision time
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 ($\text{LWP}[\text{g/m}^2]$)

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

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

<table>
<thead>
<tr>
<th>針</th>
<th>針のたば</th>
<th>針の組み合わせ</th>
<th>ごくすい</th>
<th>砲弾型</th>
<th>角柱</th>
<th>砲弾の組み合わせ</th>
<th>角柱の組み合わせ</th>
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<tbody>
<tr>
<td>丸板</td>
<td>扇形</td>
<td>枝の付いた角板</td>
<td>大幅六花</td>
<td>星状六花</td>
<td>樹枝状六花</td>
<td>シダ状六花</td>
<td>角板の付いた枝</td>
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<tr>
<td>三花</td>
<td>四花</td>
<td>上下組合せ六花</td>
<td>シダ状十二花</td>
<td>広幅十二花</td>
<td>形の整わない六花</td>
<td>立体六花</td>
<td>立体放射状</td>
</tr>
<tr>
<td>つづみ型 (角柱と枝)</td>
<td>つづみ型 (段々つづみ)</td>
<td>角柱の付いた砲弾</td>
<td>樹枝の付いた砲弾</td>
<td>不規則な集合 (粉雲)</td>
<td>交叉した角板</td>
<td>形が定まらない雲 (氷のかけら状)</td>
<td>(雲粒付き)</td>
</tr>
<tr>
<td>雲粒の付いたいろいろな結晶</td>
<td>雲粒の付いた厚い板</td>
<td>あられ状雪 (六花状)</td>
<td>あられ状雪 (かたまり状)</td>
<td>あられ (六花状)</td>
<td>あられ (かたまり状)</td>
<td>あられ (円錐状)</td>
<td></td>
</tr>
</tbody>
</table>

中谷字吉郎『Snow Crystals』 (1954) による

Araki (2014)「雲の中では何が起こっているのか」

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

rimed dendrite

graupel
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**

IN: Freezing temperature strategy

Can account for homogeneous/condensation/immersion freezing
Mass–Dimension

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

-14 -8 -2
mass log10([kg])

-6 -4 -2
maximum dimension log10([m])

-14 -8 -2

All

Graupel

Snow

Ice

ice spheres
hail (M96)
lump graupel (M96)
densely rimed dendrites (M96)
aggregates (M96)
hexagonal columns (small) (M96)
hexagonal columns (middle) (M96)
hexagonal columns (big) (M96)
hexagonal plates (M96)
broad–branched crystals (small) (M96)
broad–branched crystals (big) (M96)
vapor spheres
More result of cumulonimbus simulation is available from

SGS turbulence modeling

Turbulence affects cloud microphysics in various ways. Influence onto collision-coalescence 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

recent research software (re)developments:

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

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