Homework 5

Monte Carlo scheme for the stochastic coalescence of cloud droplets

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The mechanism responsible for precipitation in warm (i.e., ice-free) clouds is collision-coalescence among cloud droplets. Collisions may occur through differential response of the droples to gravitational, electrical, or aerodynamic forces. Here we focus on gravitational effects because they predominate in clouds. Our task is to elaborate a computer program for stochastic simulations of the collision-coalescence process induced by gravity. The program will be based on the Monte Carlo scheme developed by [Shima *et al.*, *Q. J. R. Meteorol. Soc.* **135** (2009)].

Gravitational coalescence probability: primitive model. Let P_{jk} denote the probability that the droplets with labels j and k inside the cloud volume V will coalesce in a short time interval $(t, t+\Delta t)$. For a "well-mixed" cloud, P_{jk} is given by the ratio of the *coalescence volume*, which j and k sweep out relative to each other during $(t, t+\Delta t)$, to the total cloud volume V:

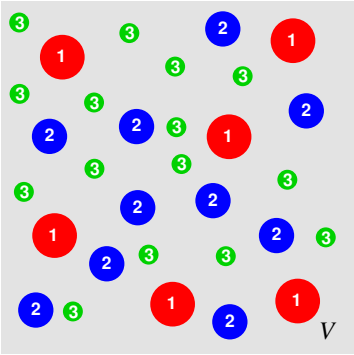
$$P_{jk} = E_{jk}\,\pi(r_j + r_k)^2 |u(r_j) - u(r_k)| \Delta t / V, \tag{1}$$

where r_j and r_k are the radii of the droplets, $u(r)$ is the r-dependent terminal sedimentation velocity. E_{jk} is the coalescence efficiency. It accounts for the fact that the coalescence volume will differ (e.g., due to hydrodynamic interaction effects) from the geometric sweep-out volume.

Super-droplets method. In cloud simulations, the volume V typically contains $O(10^{11}-10^{14})$ droplets. This makes tracking of all individual cloud droplets impossible. To cope with this limitation, we assume the volume V contains much less "computational droplets" called **super-droplets**. Each super-droplet (labeled i, with $i \in I = \{1, \ldots, \mathcal{N}\}$), is a collection of ξ_i identical **real droplets** with radius r_i (ξ_i is called the multiplicity of the ith super-droplet). Then V contains in total

$$N_r = \sum_{i=1}^{\mathcal{N}} \xi_i,$$

real droplets. We refer to (ξ_i, r_i) as the **state** of the ith super-droplet. We assume the real droplets of each super-droplet are "well-mixed" throughout V. This model system is illustrated in Figure 1.



Rysunek 1: Illustrative model system comprised of $\mathcal{N} = 3$ super-droplets with multiplicities $\xi_1 = 6$, $\xi_2 = 10$, and $\xi_3 = 15$, representing $N_r = 31$ real droplets.

The probability $P_{jk}^{(\mathrm{SD})}$ that the droplets of the super-droplets j and k inside V will coalesce in a short time interval $(t, t + \Delta t)$ may be written in terms of P_{jk}, namely,

$$P_{jk}^{(\mathrm{SD})} = \max(\xi_j, \xi_k) P_{jk}. \tag{2}$$

Monte Carlo scheme. A scheme to simulate the stochastic coalescence of the pair (j, k) of super-droplets involves two steps: (a) draw a random number ψ, uniformly distributed in the interval $[0, 1)$; (b) evaluate P_{jk} at time t. If $P_{jk} > \psi$, then the pair (j, k) coalesces at time $t + \Delta t$.

The pair (j, k) of super-droplets will change their states after coalescence according to the following rules:

(a) If $\xi_j = \xi_k$, then

$$\xi_j' = \lfloor \xi_j / 2 \rfloor, \quad \xi_k' = \xi_j - \xi_j',$$

$$r_j' = r_k' = \left(r_j^3 + r_k^3 \right)^{1/3},$$

where primes denote post-collisional values and $\lfloor x \rfloor$ gives the greatest integer less than or equal to x (floor function).

(b) If $\xi_j > \xi_k$, then

$$\xi_j' = \xi_j - \xi_k, \quad \xi_k' = \xi_k,$$

$$r_j' = r_j, \quad r_k' = \left(r_j^3 + r_k^3 \right)^{1/3}.$$

Stochastic simulation of coalescence occurring in the whole system requires application of the steps above for all possible pairs $(j,k) \in I^2$, $j \neq k$. This is inefficient if $\mathcal{N}$ is large since it yields a computational cost proportional to $\mathcal{N}^2$.

Linear sampling. The number of operations may be significantly reduced if we examine only the candidate-pairs (j,k) in the list

$$L = \{(j_1,k_1),(j_2,k_2),\ldots,(j_{\lfloor \mathcal{N}/2 \rfloor},k_{\lfloor \mathcal{N}/2 \rfloor})\},$$

that is a random permutation of the list I of the super-droplets labels (with pairs made from the front). The probability $P_{jk}^{(\mathrm{SD})}$ in Eq. (3) must be rescaled to

$$P_{jk}^{(\mathrm{SD,LS})} = \frac{\mathcal{N}(\mathcal{N}-1)}{2\lfloor \mathcal{N}/2 \rfloor} P_{jk}^{(\mathrm{SD})}, \tag{3}$$

that is, the probability $P_{jk}^{(\mathrm{SD})}$ was devided by the decreasing ratio of pair number.

Output. To characterize the time evolution of the collision-coalescence process, we monitor the following quantities:

1. Droplet number density ($n \equiv N/V$),

$$n = \frac{1}{V}\sum_{k=1}^{\mathcal{N}} \xi_k; \tag{4}$$

2. Precipitation rate (R),

$$R = \frac{\pi}{6}\frac{1}{V}\sum_{k=1}^{\mathcal{N}} \xi_k (2r_k)^3 u(r_k); \tag{5}$$

3. Radar reflectivity factor (Z),

$$Z = 10\log_{10}\left(\frac{z}{z_0}\right) \quad [\mathrm{dBz}], \tag{6}$$

where

$$z = \frac{1}{V}\sum_{k=1}^{\mathcal{N}} \xi_k (2r_k)^6, \tag{7}$$

and $z_0 = 1\ \mathrm{mm}^6\ \mathrm{m}^{-3}$.

Building the simulation code and setup. Elaborate the simulation code according to the following steps:

1. Set the coalescence cell volume $V = 10^6$ m^3 and the initial number density of droplets $n_0 = 100$ cm^{-3}. The initial number of super-droplets $\mathcal{N}$ is a variable simulation parameter. Set $\mathcal{N} = 100$ for preliminary tests. The initial multiplicity is the same for all super-droplets and is given by $\xi_i = n_0 V/\mathcal{N}$ $(i = 1, \ldots, \mathcal{N})$. The time step Δt is a variable simulation parameter. Set $\Delta t = 0.01$ s for preliminary tests.

2. Set an initial radius distribution by assuming that the droplet volume $v = (4\pi/3)r^3$ follows an exponential distribution,

$$f(v) = \frac{1}{\bar{v}} \exp\left(-\frac{v}{\bar{v}}\right), \quad (v \geq 0), \tag{8}$$

   where $\bar{v} = (4\pi/3)\bar{r}^3$. Set $\bar{r} = 30.531$ μm. Develop a subroutine to randomly generate the volumes $\{v_i\}$ of the super-droplets by *inverse transform sampling*. Having $\{v_i\}$ evaluate the corresponding radii $\{r_i\}$.

3. Develop a subroutine to evaluate the terminal sedimentation velocity,

$$u(r) = \alpha r^\beta,$$

   of cloud droplets according to a chosen parametrization (α, β constants).

4. Develop a subroutine to evaluate the collision probabilities. First in the primitive model (i.e., P_{jk} in the system of real droplets), and then in the system of super-droplets (i.e, $P_{jk}^{(\mathrm{SD})}$ for sampling over the whole set of colliding pairs and $P_{jk}^{(\mathrm{SD,LS})}$ for the linear sampling).

5. Develop a subroutine to compute the change of the super-droplets state after a coalescence event. How should we proceed when $\xi_j = \xi_k = 1$ (what results in $\xi_j' = 0$ and $\xi_k' = 1$ after coalescence)?

6. Develop a subroutine to compute the output variables: droplet number density (n), precipitation rate (R), and radar reflectivity factor (Z).

7. Combine all the subroutines above in the Monte Carlo scheme.