Particle-based coalescence/aggregation: Rigorous evaluation and comparison with bin model solutions

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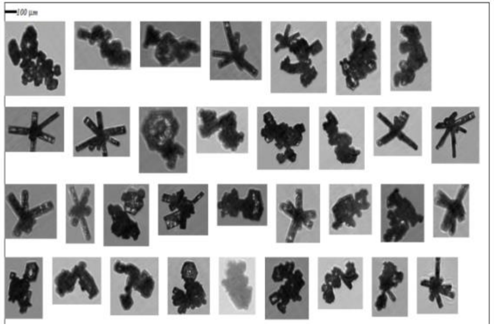
Particle collisions in clouds/aerosol

Terminology:

collision + *cohesion* = *collection*

- Called *coalescence* in warm clouds
  Important process for rain formation
- Called *aggregation* in ice clouds
  Creates irregular crystal shapes affecting fall speed, deposition growth rates and radiative properties
- Called *coagulation* for aerosol particles
- Called *riming*, when ice particles and liquid drops merge

This talk focuses on the numerical treatment, not really on the physics, so the above terms are more or less synonymously used here.



Gallagher et al, 2012

Collision probability

P_{ij} is the probability that a single droplet with mass m_i collides with a single droplet of mass m_j inside a small volume δV and short time interval δt

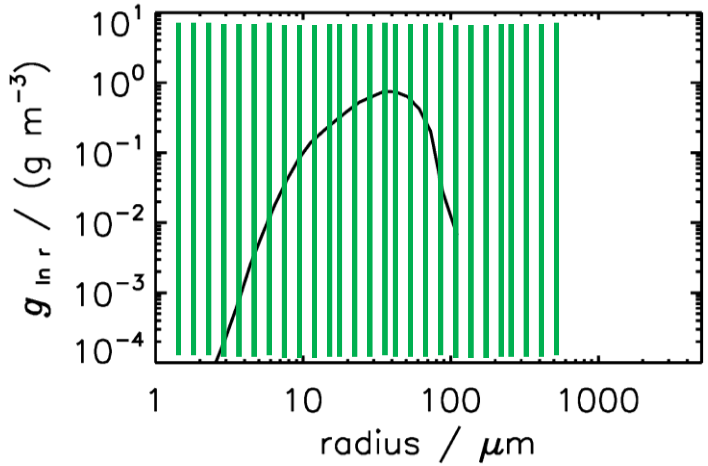
$$P_{ij} = K_{ij}\ \delta t\ \delta V^{-1}$$

The kernel K_{ij} contains all the physics.
The expected value of the number of collisions for concentrations n_i and n_j of such droplets:

$$n_{coll} = K_{ij} * n_i * n_j * dt$$

Gillespie, 1972

Numerical procedure in a bin model

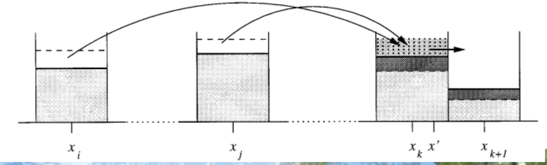


- Average number of collisions between droplets of bin i und j:

$$n_{coll} = K_{ij} * n_i * n_j * dt$$

- After time dt:
  - bin i: $n_i = n_i - n_{coll}$
  - bin j: $n_j = n_j - n_{coll}$
  - bin k: $n_k = n_k + n_{coll}$
  - Choose bins k such that $m_k = m_i + m_j$
- Do it for all bin combinations with $i < j \leq N$
- Next time step

Established algorithms exist *(Bott, 1998, Wang, 2007, Simmel, 2002).*



Lagrangian microphysics

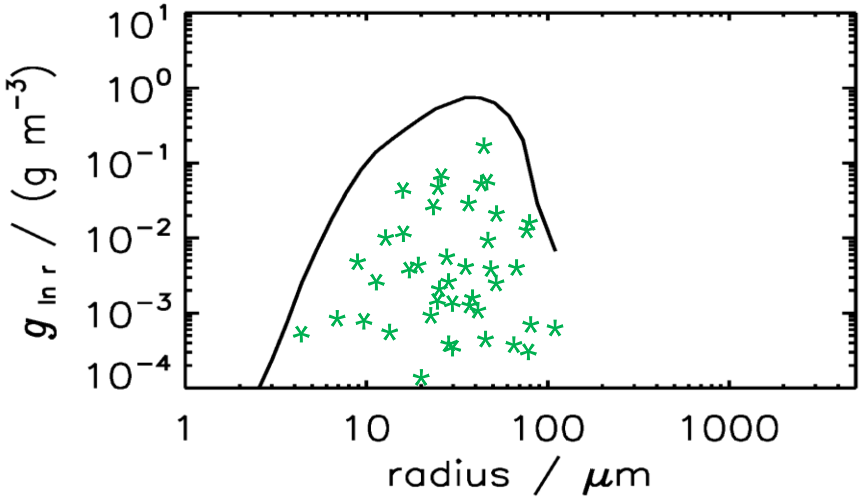
Terminology:

- particle based microphysics =
  Lagrangian cloud microphysics (LCM) =
  superdroplet method

- Each superdroplet or SIP (simulation particle) represents
  v_i identical droplets of mass m_i

- v_i is called multiplicity or weighting factor

Lagrangian microphysics



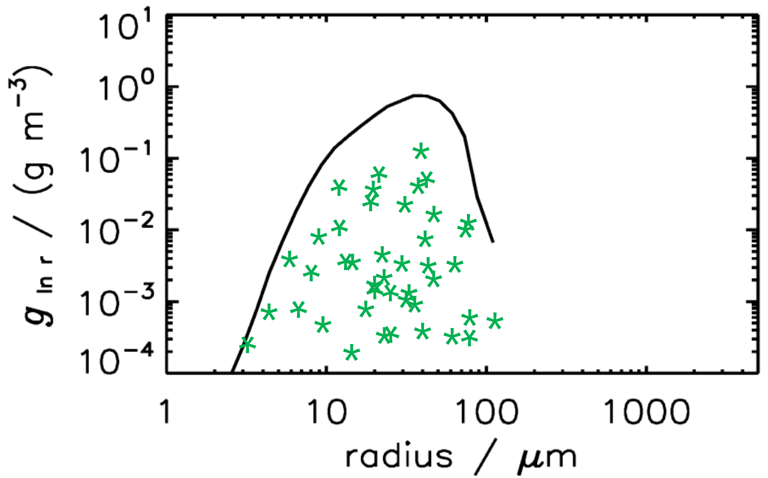
Each * shows a SIP with a certain v_i and m_i

This shows one possible SIP ensemble that approximates the size distribution.

Define volume dV over which the droplets of a SIP are spread out and assumed to be well mixed.
(*usually take dV of Eulerian host model*)

Numerical procedure in a particle-based approach

More or less analogous to bin models!? Let‘s see …



- number of collections involving droplets from SIP i and j:

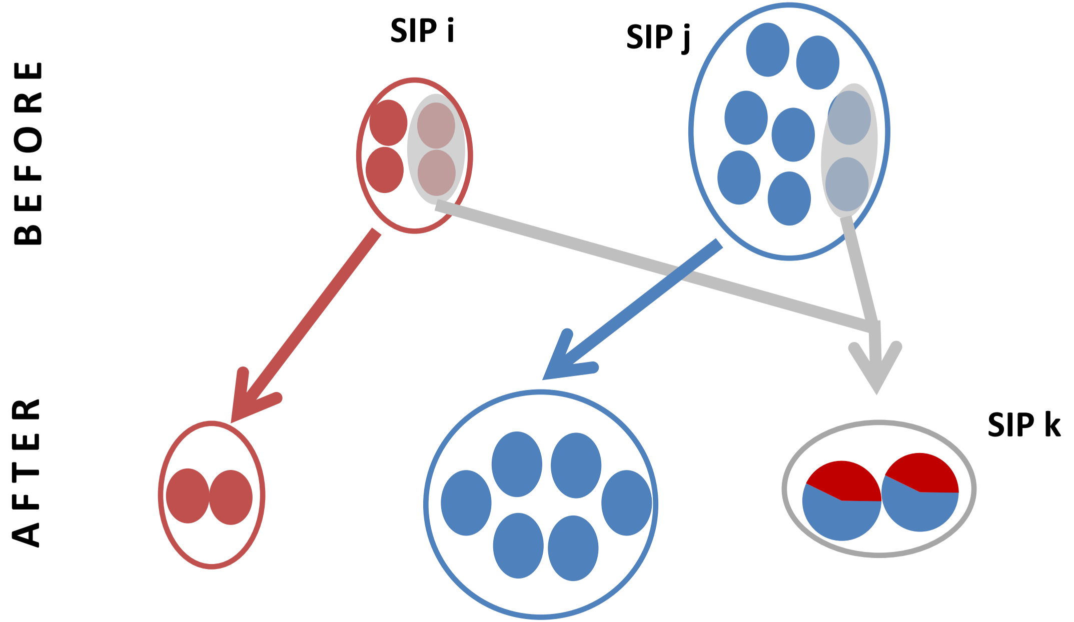
$$\nu_{coll} = K_{ij} * \nu_i * \nu_j * dt * dV^{-1}$$

- After time dt:
  - SIP i: $\nu_i = \nu_i - \nu_{coll}$
  - SIP j: $\nu_j = \nu_j - \nu_{coll}$
  - SIP k: $\nu_k = \nu_{coll}$ and $m_k = m_i + m_j$
- Do it for all SIP combinations with $i < j \leq N$
- Next time step

SIP k does not exist, must be created! Not feasible!!
What solutions do exist?

Example with $v_i = 4$, $v_j = 8$ and $v_{coll} = 2$
assume $m_i < m_j$

Hypothetical algorithm



reduce v_i by v_{coll}

reduce v_j by v_{coll}

new SIP with
$v_k = v_{coll}$ and $m_k = m_i + m_j$

Review of aggregation/collection algorithms in LCM

Avoid generating new SIPs! Various ideas and approaches exist:

1. Remapping-Algorithm (*Andrejczuk et al, 2010*)

2. Average Impact Algorithm (*Riechelmann et al, 2012*)

3. All-Or-Nothing-Algorithm (*Shima et al, 2009, Sölch & Kärcher, 2010*)

The three algorithms have been investigated in detail in a boxmodel framework:

Unterstrasser, Hoffmann & Lerch: Collection/aggregation algorithms in Lagrangian cloud microphysical models: Rigorous evaluation in box model simulations, GMD, 2017

Example with v_i = 4, v_j = 8 and v_{coll} = 2
assume $m_i < m_j$

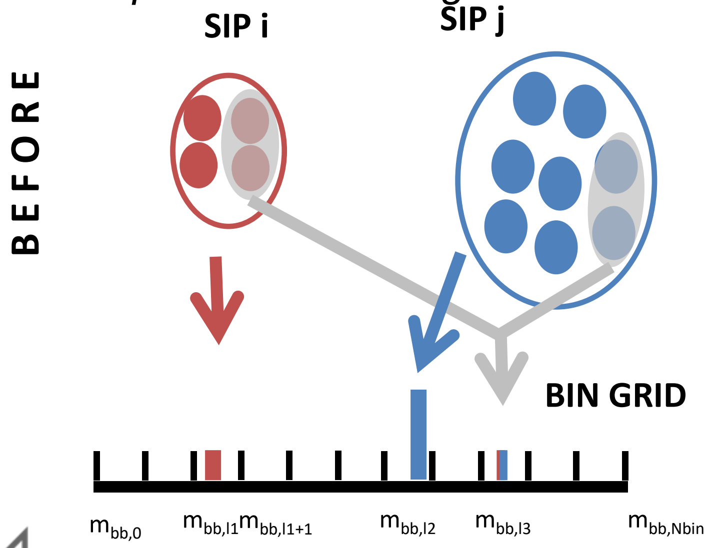
Remapping Algorithm

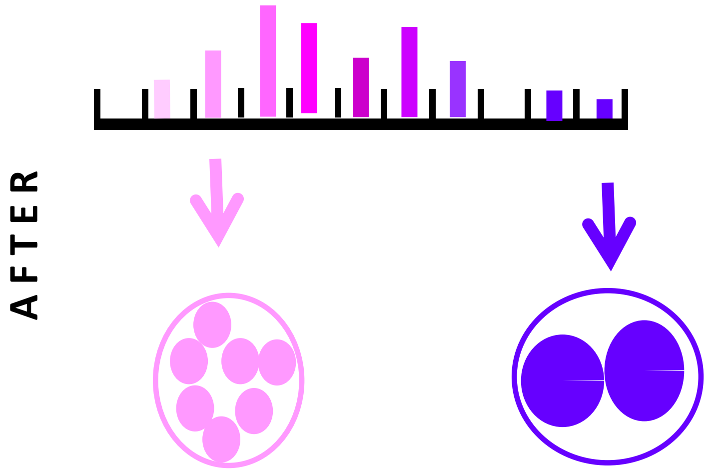
Avoid generating new SIPs! How?

Merge similar SIPs! Use temporary bin grid to sum up the contributions.

Generate new SIP ensemble after each time step. One SIP per bin.

Conceptual disadvantage in full simulations: loose SIP history, trajectory information, ...





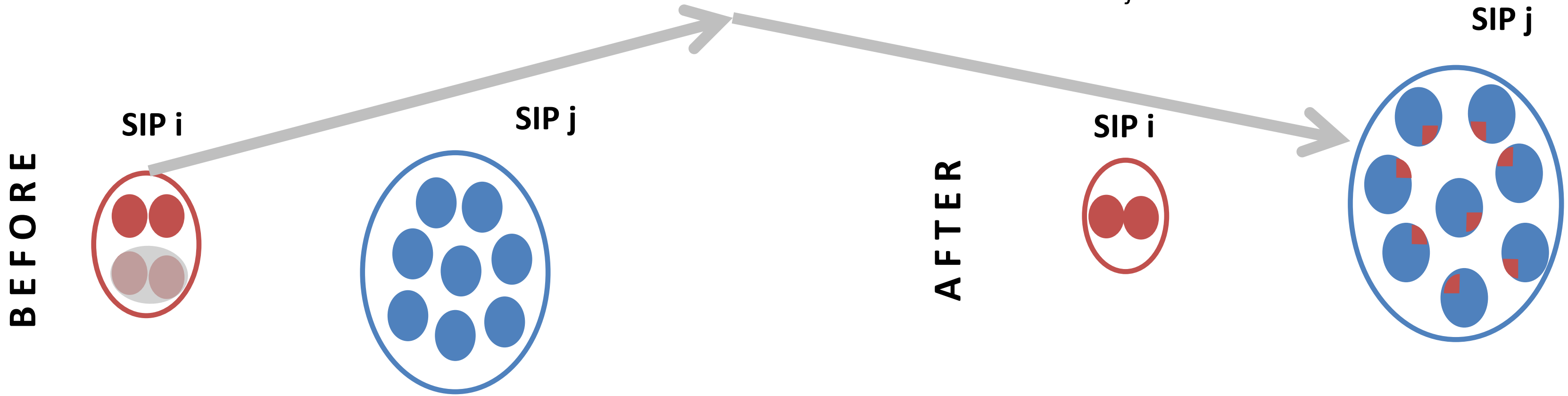
Example with $v_i = 4$, $v_j = 8$ and $v_{coll} = 2$
assume $m_i < m_j$

Average Impact Algorithm

Avoid generating new SIPs! How?

Account for mass transfer from SIP i to SIP j (assume $m_j > m_i$).

Possible problem: Called „Average impact“ because transfered mass is distributed among all droplets of SIP j. No droplets with mass $m_i + m_j$ are created.

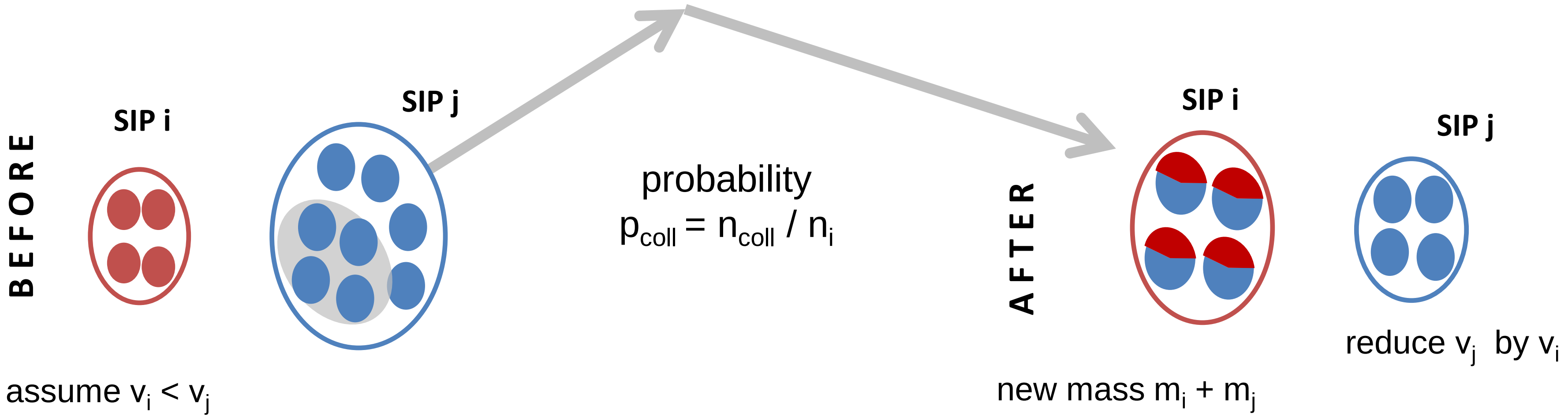


New mass
$m_j + (v_{coll} / v_j) * m_i$

Example with $v_i = 4$, $v_j = 8$ and $v_{coll} = 2$
assume $m_i < m_j$

All-Or-Nothing Algorithm

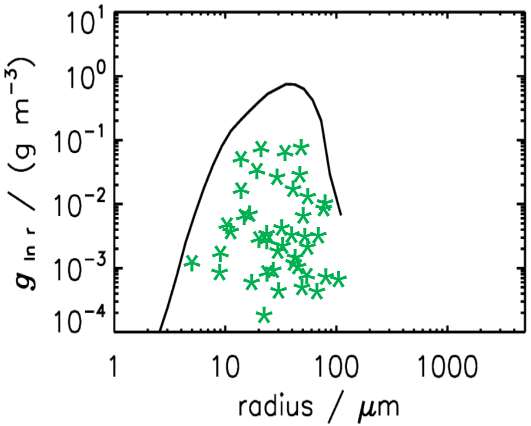
Avoid generating new SIPs! How?
Do not always perform a collection event in the model.
Define that all v_i droplets of SIP i are collected instead of n_{coll}.
Drawback: probabilistic approach requires averaging over realisations (we use 50)



Rigourous evaluation in box model simulations

Setup

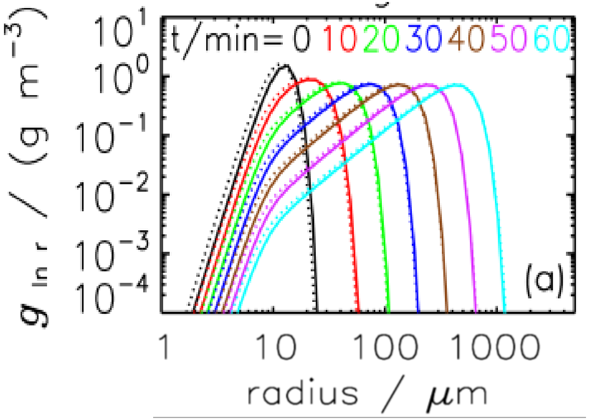
- One grid box
- Aggregation/collection is the only process
- Tests with Golovin kernel and Long/Hall kernel
- Start with prescribed **continuous** size distribution (SD)
  In a particle-based approach this offers an additional degree of freedom!
  There is not a unique SIP representation of a given SD



Example with Golovin kernel

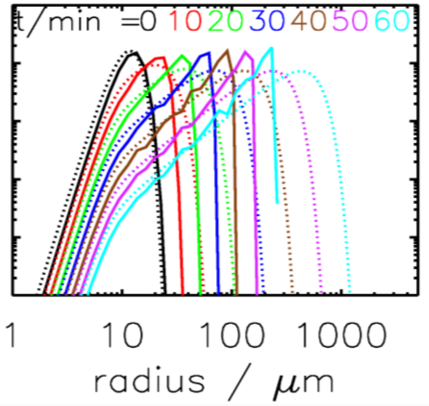
Golovin-Kernel („sum of masses“): analytical solution (dotted lines)

Remapping



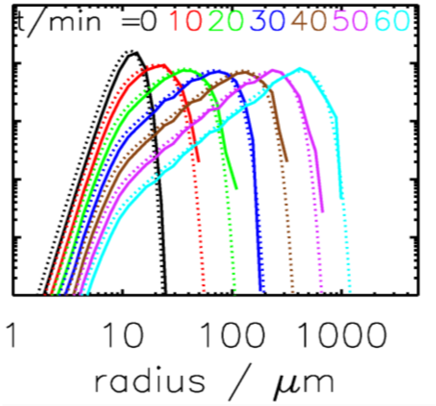
perfect

Average Impact



gets stuck

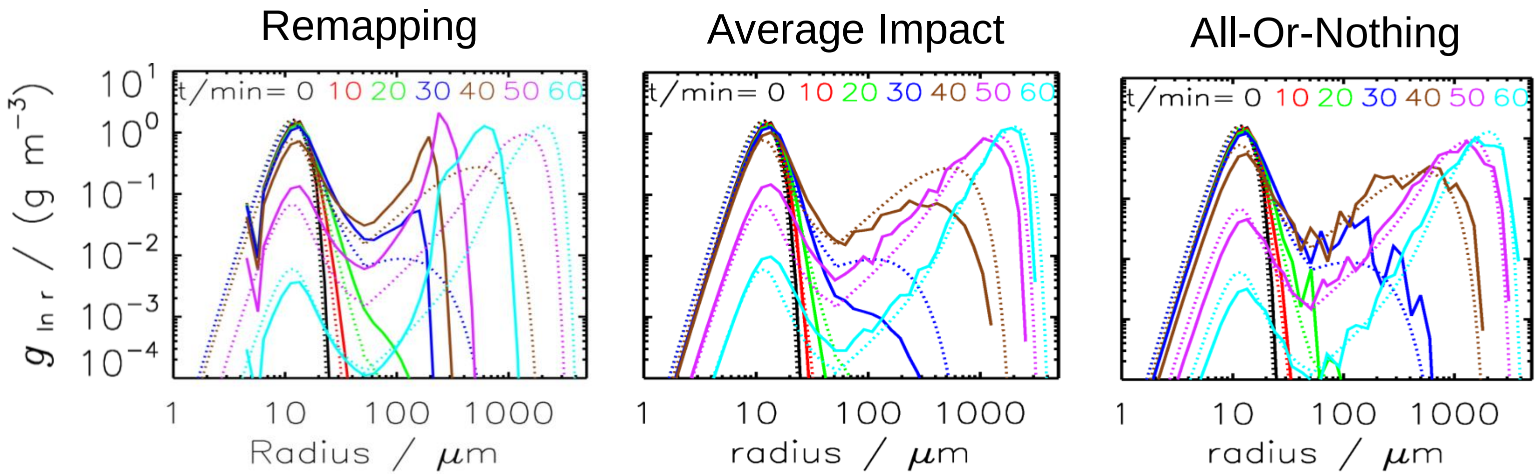
All-Or-Nothing



very good

Example with Long kernel

Long-Kernel: benckmark bin model solution by Wang et al, 2007 (dotted lines)



gets stuck

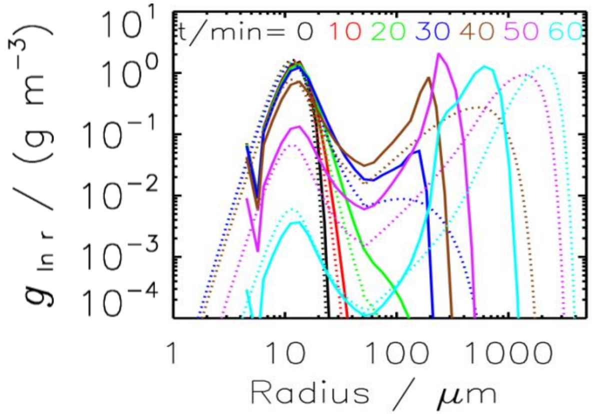
(surprisingly) good

very good

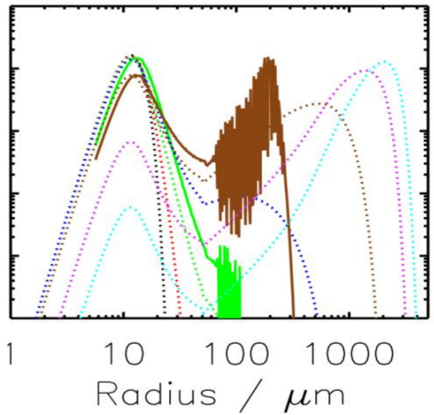
Remapping Algorithm in detail

Why does the Remapping algorithm get stuck with the **Long-Kernel**?

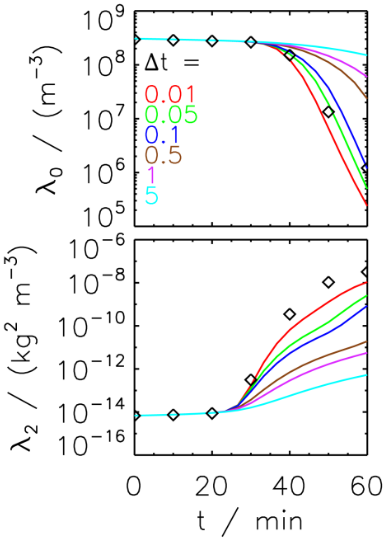
coarse plot



Actually it looks like



Stable only for tiny dt



Remapping Algorithm in detail

Why does the Remapping algorithm get stuck with the **Long-Kernel**?

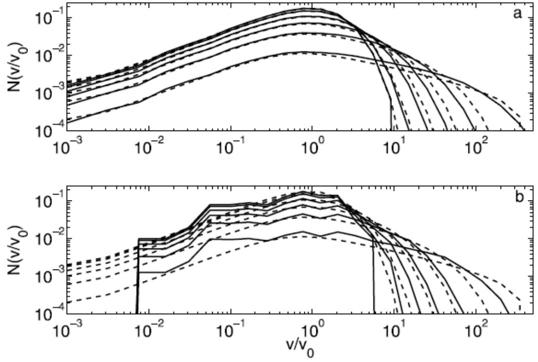


Figure 11. Initial distribution and solutions for times 69, 233, 450, 790, and 1500 s for the Golovin kernel (dashed line) and LCM scheme (solid line). (a) Solution with 100 parcels initially averaged over 100 realizations and (b) solution for 100 parcels initially.

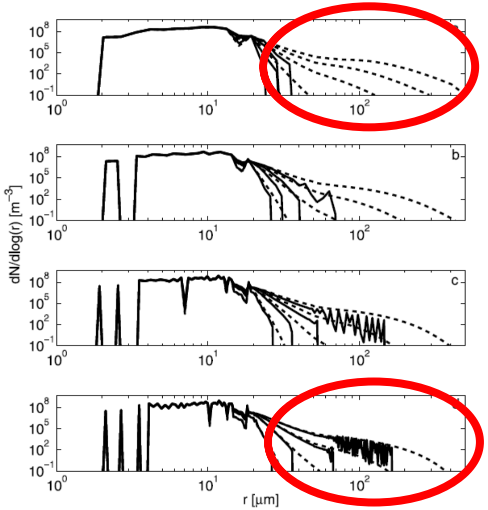
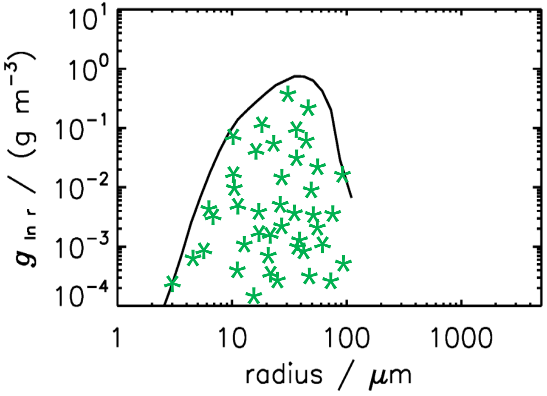


Figure 13. Solutions after 200, 800, 1400, and 2000 s for hydrodynamic kernel with Long collision efficiency for Bott scheme (dashed line) and LCM scheme (solid line) for (a) 30 bins, (b) 60 bins, (c) 120 bins, and (d) 240 bins.

Verification exercises by Andrejczuk et al, 2010

Effect of SIP ensemble properties

Additional degree of freedom: SIP ensemble generation for a prescribed SD



„nice“ SIP ensemble: use temporary bin grid, draw one SIP from each bin with well-defined m_i and v_i

„equal weights“ SIP ensemble: all nr_{SIPs} SIPs have the same weight N_{tot}/nr_{SIPs}. Draw mass according to F^{-1}, where F is cumulative SD.

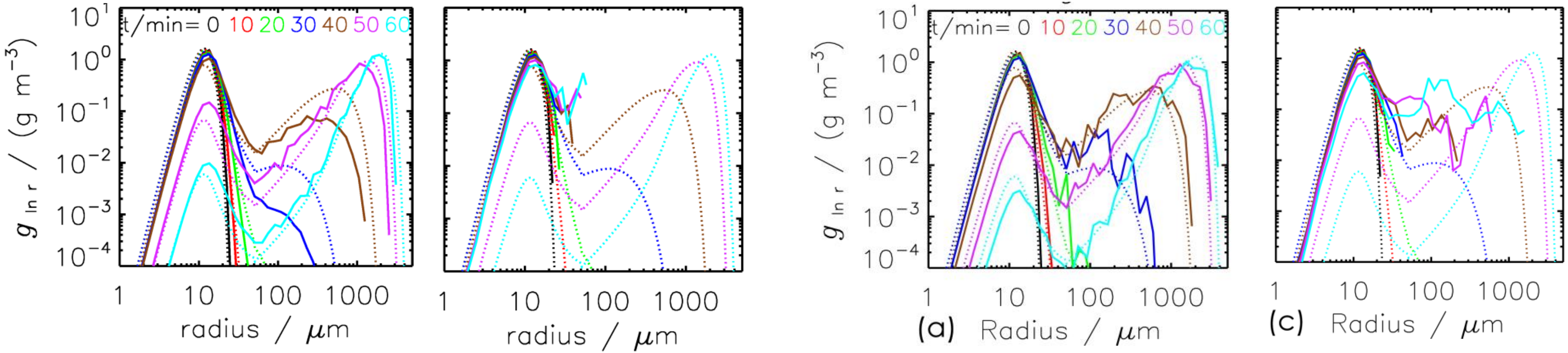
3D LCM simulations are often initialized with equal weights SIPs

Effect of SIP ensemble properties

Long kernel example

Average Impact Algorithm **All-Or-Nothing Algorithm**

„nice“ SIP ensemble equal weights „nice“ SIP ensemble equal weights

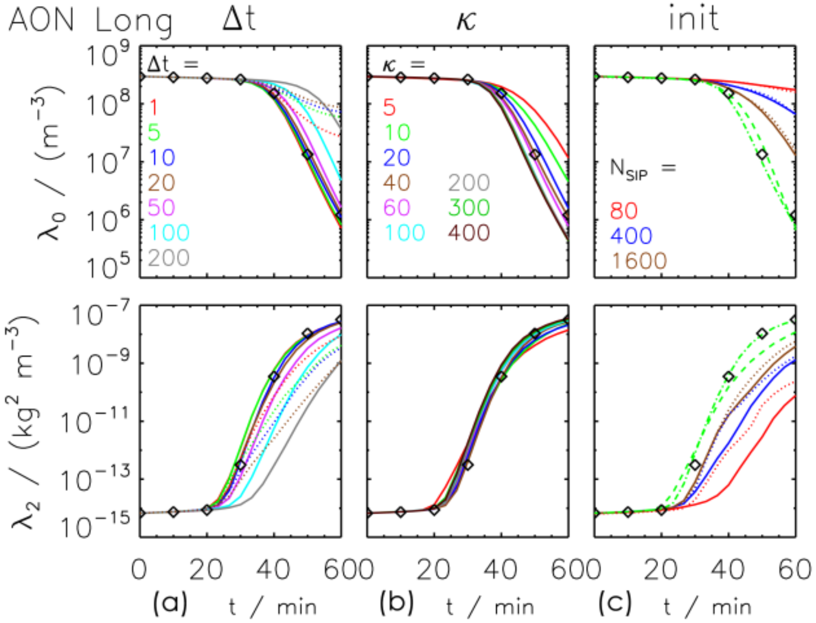


Algorithms perform best for „nice“ SIP ensemble.
SIPs with small weights are not really relevant for other processes like condensation, but are essential for a good performance of aggregation/collection algorithms.

How many SIPs are needed?

And what about the time step? Results for **All-Or-Nothing (AON) Algorithm**

nrSIPs = 5 * κ



Left: dt < 50s seems to suffice!

Middle: For a „nice“ SIP ensemble, 200 SIPs are enough. For a „good“ second moment fewer SIPs are sufficient.

Right: no quantitative agreement possible if a equal weights SIP ensemble is used.

Shima et al, 2009 in the pioneering work used „equal weights“ and reached convergence only for >O(10^5) SIPs.

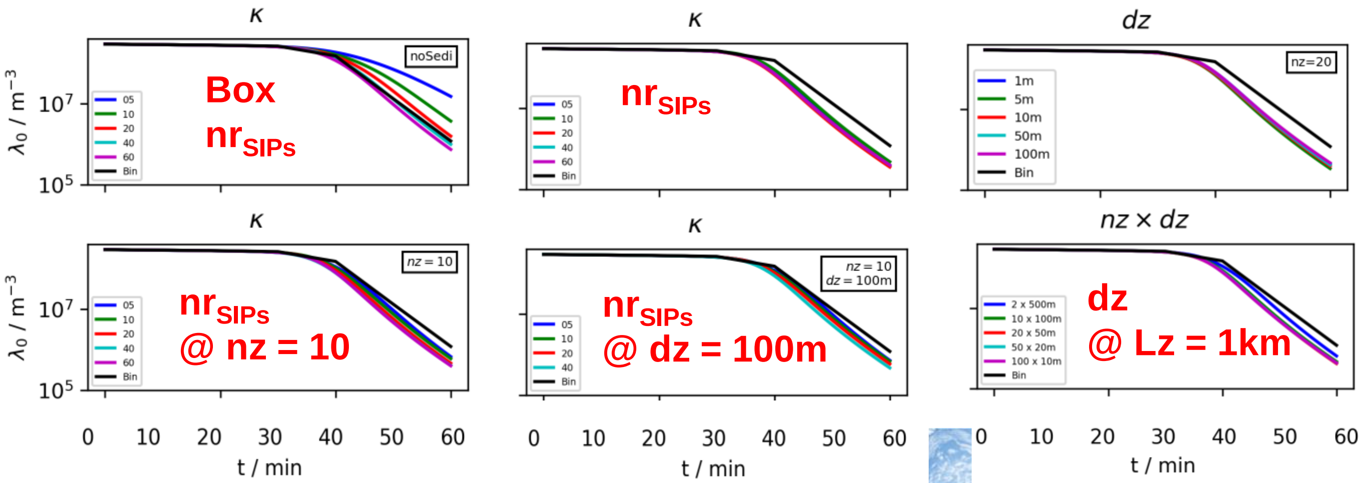
First Column model test case

periodic boundary conditions and homogenous initial vertical profile

⇒ Expect similar evolution in all grid boxes (GB) as in the box model before

⇒ Difference bin model vs. AON:

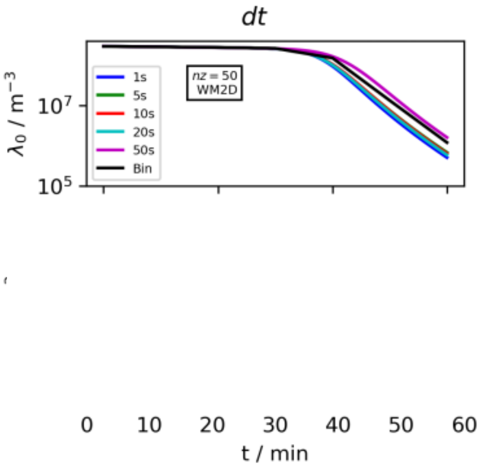
- deterministic bin model -> identical results in each GB
- in AON lucky droplets can collect droplets from several GBs
- important finding: less SIP are required for convergence in column model

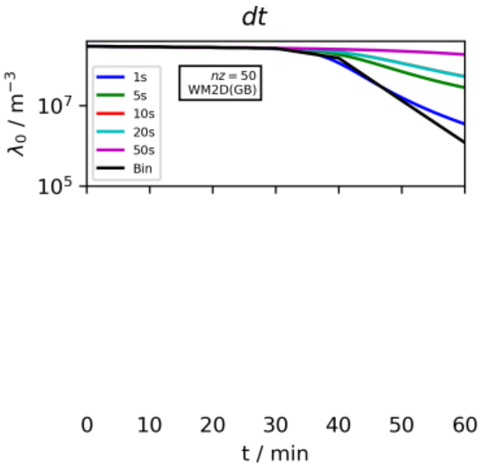


Default setup:
nz = 50 grid boxes
dz = 10m
dt = 10s
20 realisations
200 SIPs/GB

AON version with explicit overtakes

- use vertical position of SIP in aggregation algorithm (version of Sölch & Kärcher, 2010)
- droplets of a SIP are assumed to be well mixed on plane $z=z_i$ („concentration“ ν_i/dA)
- explicitly compute if a SIP i overtakes SIP j during a time step
- adapt hydrodynamical kernel expression accordingly





$$K(r,r') = \pi (r+r')^2 \cancel{|v_{sed}(r) - v_{sed}(r')|} E_c(r,r')$$

$$\nu_{coll}' = \pi (r_i + r_j)^2 \, \nu_i \, \nu_j \, \Delta A^{-1} E_c(r,r')$$

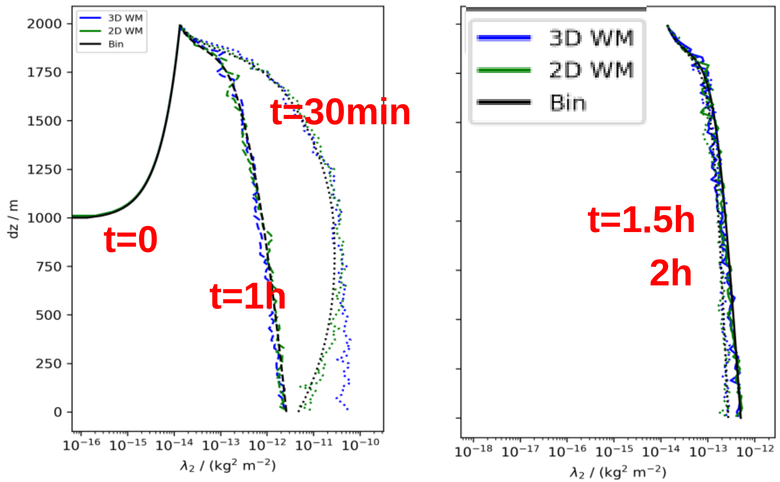
- gives similar results for uniform profile (serves as verification exercise)
- may be more realistic than regular AON for non-uniform profiles with size separation

Bin model: Bott algorithm for KCE + MPDATA advection for sedimentation equation

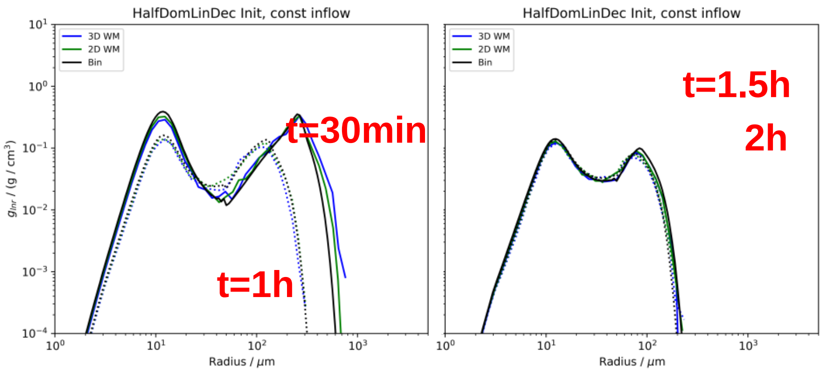
Non-Uniform Profile

Linearly decaying profile in upper half of 2km column; constant inflow at top BC

Profile of second moment



Size distribution

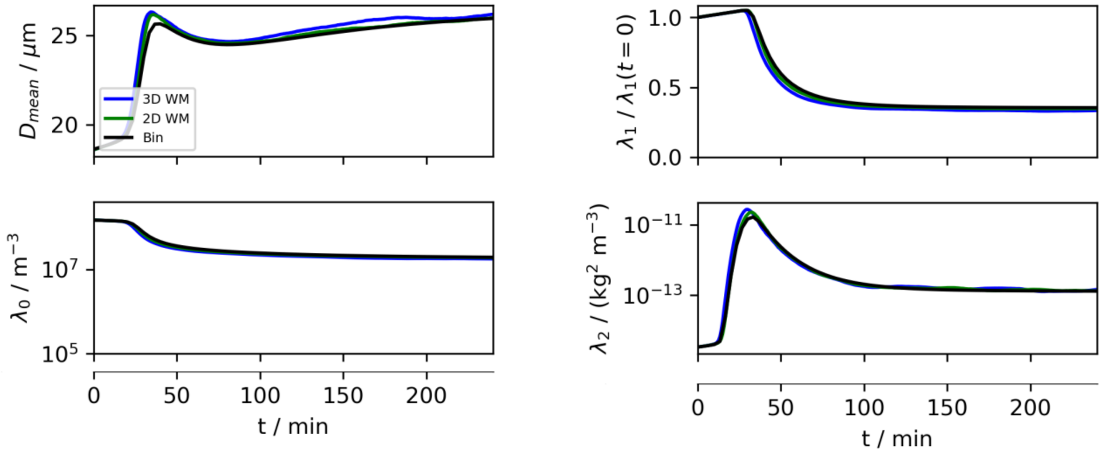


Bin model: Bott algorithm for KCE + MPDATA advection for sedimentation equation

Non-Uniform Profile

Linearly decaying in upper half of 2km column, constant inflow

Temporal evolution of mean diameter and moments 0, 1 and 2



Despite different numerical treatment of sedimentation and aggregation/collection, the perfect agreement between Eulerian and Lagrangian approach is promising

Summary

- Rigorous box model evaluation of three particle-based aggregation/collection algorithms
- The probabilistic All-Or-Nothing (AON) Algorithm (Shima et al, 2009, Sölch & Kärcher, 2010) performs best.
- Performance analysis of algorithms more complex than in bin models, as the SIP representation of a given continuous SD is not unique.
- AON can also be used for more fundamental research (see also e.g. Dziekan & Pawlowska, 2017)
- Column model application: AON convergence is not really a critical issue
- More realistic AON version with explicit overtakes works equally well
- AON approved for 3D model simulations