Stochastic coalescence in Lagrangian cloud microphysics[1]

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[1] P. Dziekan and H. Pawlowska *Atmospheric Chemistry and Physics* 2017, vol. 17.22, pp. 13509-13520

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Description of coalescence

Levels of description of collision-coalescence of droplets, listed in the order of decreasing precision:

- Microscopic - deterministic tracking of droplet positions (DNS).
- Mesoscopic - stochastic Markovian process assuming well-mixed volume (master equation, Gillespie algorithm).
- Macroscopic - deterministic equation for the mean value of the stochastic mesoscopic process; requires additional assumptions (Smoluchowski equation, also known as stochastic coalescence equation, SCE).
- Bulk parametrizations.

Where does the Super-Droplet Method (SDM) fit in?

Super-Droplet Method[2] is one of Lagrangian, particle-based methods developed in the last decade to study cloud microphysics. The idea is to model physical processes on a relatively small number of computational droplets, each representing a large number of real droplets. The collision-coalescence procedure used in SDM is based on the following simplifications:

- Coalescence volume is well-mixed.
- Linear sampling of collision pairs.
- Each computational droplet represents many real droplets - decreased statistical sample.
- Computational droplets collide in an all-or-nothing manner.

[2] S. Shima *Q. J. R. Meteorological Society* 2009, vol. 135(642), pp. 1307-1320

"One-to-one" simulations

To test precision of SDM, we start with simulations in which one computational droplet represents only one real droplet, what we call "one-to-one" simulation. By comparing "one-to-one" simulations with the master equation we show, that they are at the same level of precision:

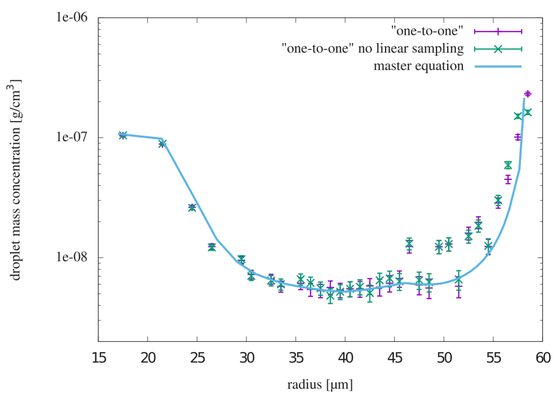

Figure 1: Mean droplet size spectrum from an ensemble of "one-to-one" simulations with and without linear sampling. Solution of the master equation is taken from Alfonso and Raga 2017[3]

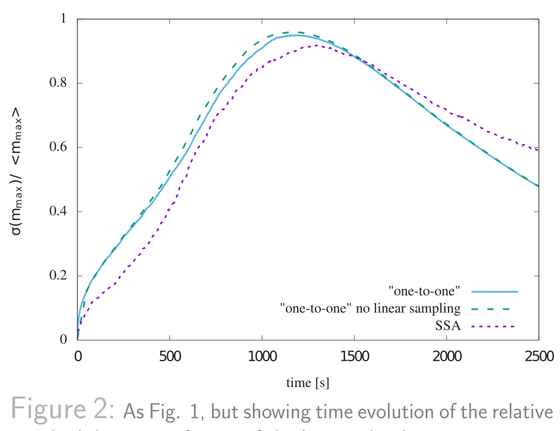

Figure 2: As Fig. 1, but showing time evolution of the relative standard deviation of mass of the largest droplet.

[3] L. Alfonso and G. B. Raga *Atmospheric Chemistry and Physics* 2017, vol. 17(11), pp. 6895-6905

SDM - mean autoconversion time

"One-to-one" simulations are used to test if SDM gives correct mean results. Results depend on size of the coalescence cell parametrized by N_0 - initial number of droplets in the cell.

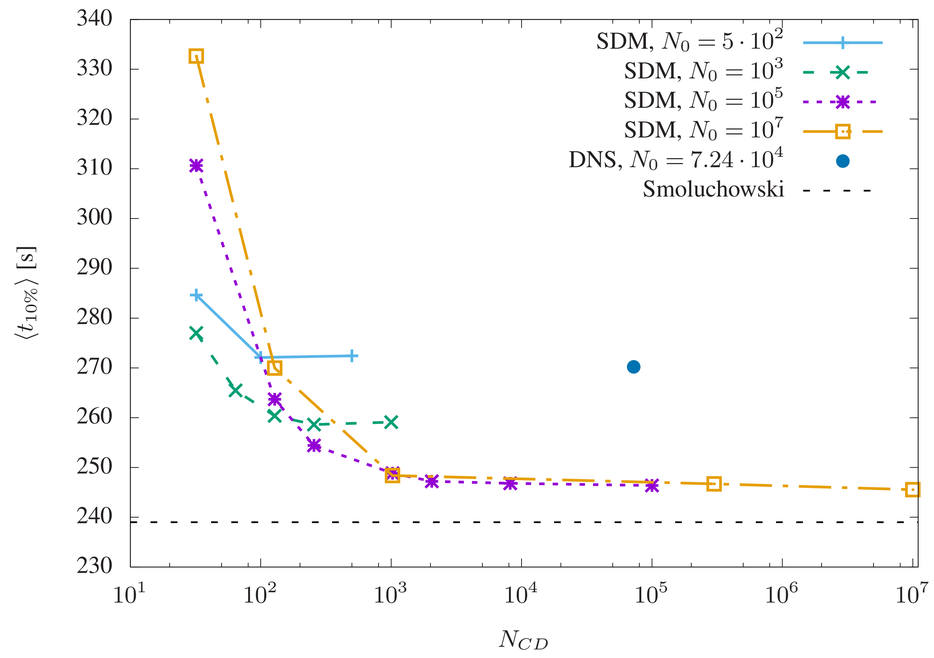

Figure 3: Mean autoconversion time $t_{10\%}$ (time it takes for 10% of cloud water to turn into rain water) from an ensemble of SDM simulations for different cell sizes. N_{CD} is the number of computational droplets. Rightmost point in each series comes from "one-to-one" simulations, in which $N_{CD} = N_0$. For reference, results of the Smoluchowski equation and of DNS[4] are shown.

- In "one-to-one" simulations, mean autoconversion time asymptotically decreases with increasing coalescence cell size.
- SCE predicts $t_{10\%}$ to be shorter than the asymptotic limit of the "one-to-one" simulations, probably due to numerical diffusion.
- Using few computational droplets in SDM causes delay in autoconversion: 10% (1%) delay for 100 (1000) computational droplets.
- DNS gives slower autoconversion. Probably the coalescence kernel is not right, but it could also mean that the correct size of coalescence cell is $N_0 = 500$.

[4] R. Onishi et al. *Journal of the Atmospheric Sciences* 2015, vol. 72(7), pp. 1005-1032

SDM - standard deviation of autoconversion time

Scaling of fluctuations in autoconversion time with coalescence cell size is studied using ensembles of "one-to-one" and SDM simulations.

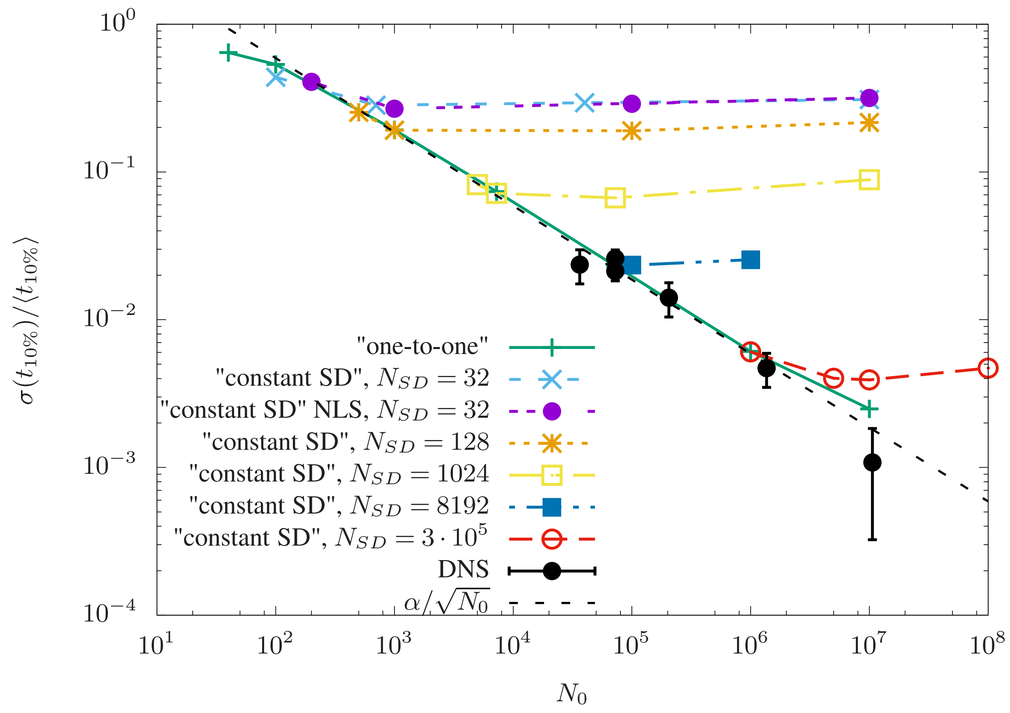

Figure 4: Relative standard deviation of the autoconversion time vs coalescence cell size. N_{SD} is the number of computational droplets (also called super-droplets) and "constant SD" denotes regular SDM. NLS stands for "no linear sampling". Dashed line with $\alpha = 6$ was fitted to "one-to-one" results. DNS results taken from Onishi et al.[4].

- DNS and "one-to-one" modeling show that relative standard deviation of autoconversion time scales with cell size as: $6/\sqrt{N_0}$.
- Using few computational droplets in SDM imposes a lower limit on the relative standard deviation.
- SDM gives correct standard deviation if $N_{SD} > N_0/9$, otherwise it gives too high standard deviation.

SCE validity

Stochastic coalescence equation (or Smoluchowski equation) gives time evolution of the mean concentration of droplets. It is derived assuming that the coalescence cell is large. Using "one-to-one" simulations we quantify exactly how large the cell needs to be.

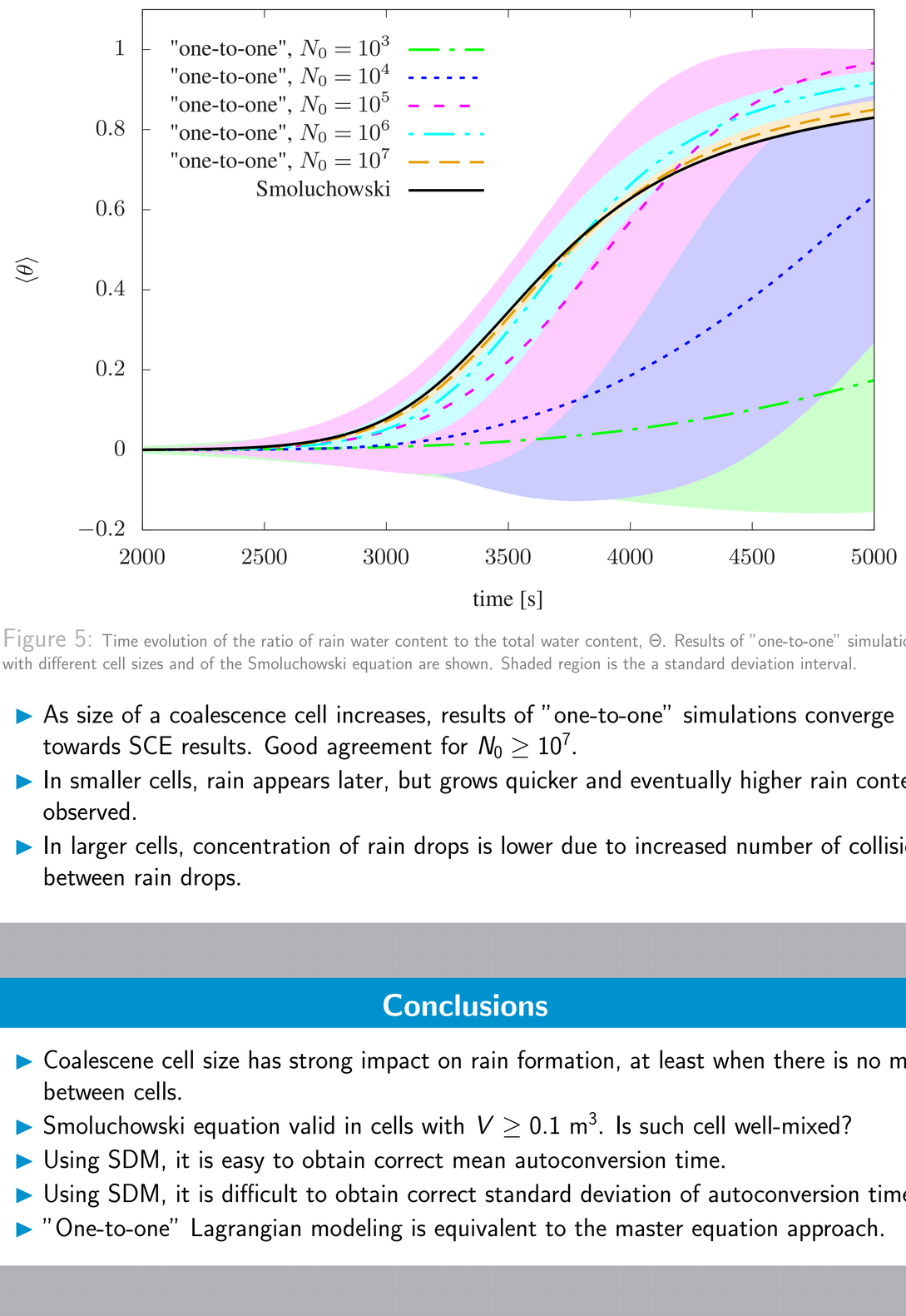

Figure 5: Time evolution of the ratio of rain water content to the total water content, Θ. Results of "one-to-one" simulations with different cell sizes and of the Smoluchowski equation are shown. Shaded region is the a standard deviation interval.

- As size of a coalescence cell increases, results of "one-to-one" simulations converge towards SCE results. Good agreement for $N_0 \geq 10^7$.
- In smaller cells, rain appears later, but grows quicker and eventually higher rain content is observed.
- In larger cells, concentration of rain drops is lower due to increased number of collisions between rain drops.

Conclusions

- Coalescene cell size has strong impact on rain formation, at least when there is no mixing between cells.
- Smoluchowski equation valid in cells with $V \geq 0.1$ m^3. Is such cell well-mixed?
- Using SDM, it is easy to obtain correct mean autoconversion time.
- Using SDM, it is difficult to obtain correct standard deviation of autoconversion time.
- "One-to-one" Lagrangian modeling is equivalent to the master equation approach.

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work financed by NATIONAL SCIENCE CENTRE POLAND