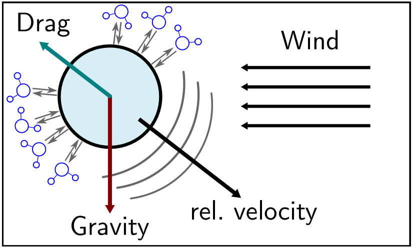
Discrete particle methods for cloud microphysics simulations



Source: World Meteorological Organization (WMO)

Jan Bohrer 21.11.2019

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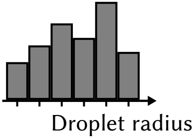
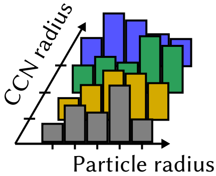
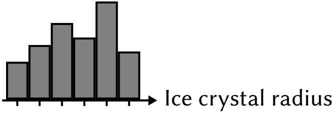
Leibniz Institute for Tropospheric Research

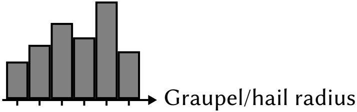
Traditional cloud models

	Single moment bulk	Double-moment bulk	1D bin model	2D bin model
Warm rain microphysics				
Cloud droplets	r_c	r_c, n_c		
Rain drops	r_r	r_r, n_r		
Ice microphysics				
Cloud ice	r_i	r_i, n_i		
Snow	r_s	r_s, n_s		
Graupel/hail	r_g	r_g, n_g		





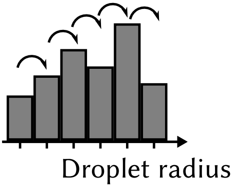




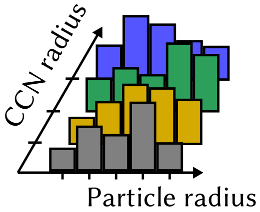
Motivated by [Grabowski *et al.* (2019), Bull. Am. Meteorol. Soc. **100**, 655]

Limitations of bin models

- Numerical diffusion



- "Curse of dimensionality"

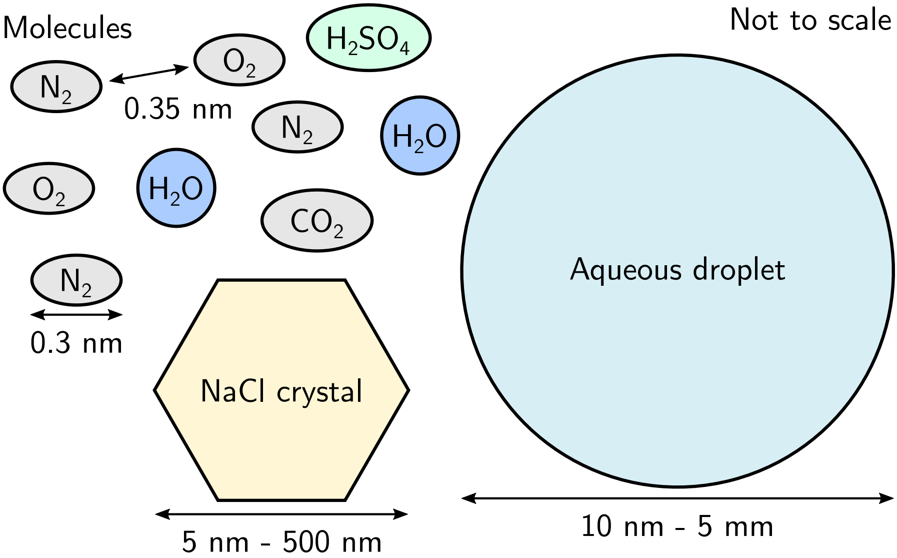


Why Lagrangian cloud models?

- No numerical diffusion in radius space
- "Curse of dimensionality" lifted
- Straightforward implementation of multicomponent chemistry
- Detailed description of ice crystals: Shape, phases, growth, ...
- Stochastic treatment of particle collisions and local turbulence

Outline

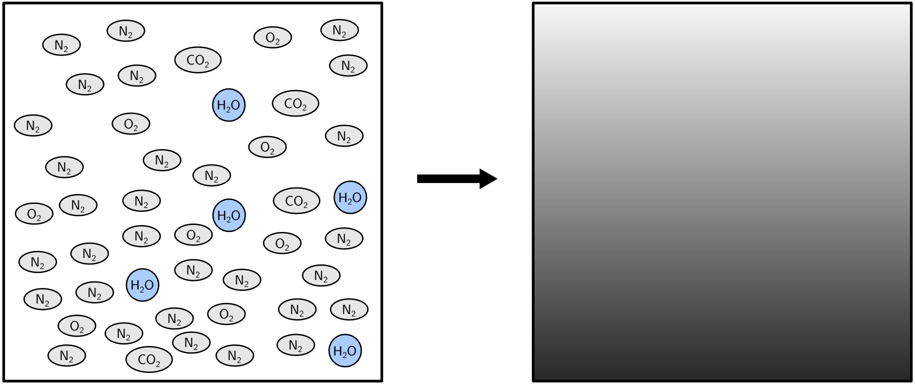
Atmospheric composition



Moist air as continuous fluid

Particle view

Continuous fluid with fields
$\rho(\boldsymbol{x})$, $p(\boldsymbol{x})$, $T(\boldsymbol{x})$, $\boldsymbol{u}(\boldsymbol{x})$



Atmospheric thermodynamics

- Ideal gas equation of state: $p = \tilde{R}_m \, \rho_m \, T$

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$$\dot{q}_{\mathrm{con}} = L_v \frac{\phi_{\mathrm{con}}}{\rho_m}$$

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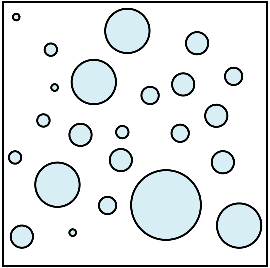
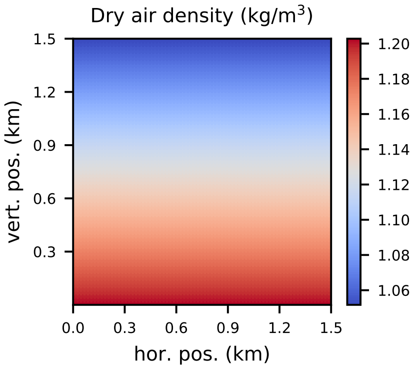


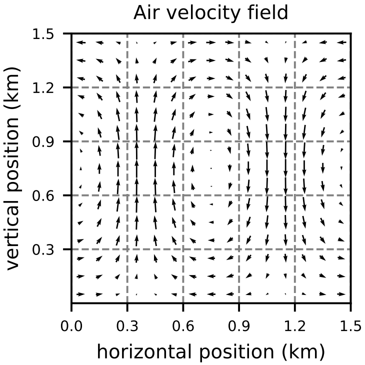
- Condensation mass rate by coarse graining:

$$\Phi = \int_V \mathrm{d}V \phi_{\mathrm{con}} = \sum_{\boldsymbol{x}_\alpha \in V} \dot{m}_\alpha$$

Atmospheric kinematic model (2D)

- Test case 1 of the international cloud modeling workshop 2012
  [Muhlbauer *et al.* (2013), Bull. Am. Meteorol. Soc. **94**, 45]





- **Stationary** dry air density and dry air mass flux:

$$\rho_{\mathrm{dry}} = \rho_{\mathrm{dry}}(z) \qquad \rho_{\mathrm{dry}}\boldsymbol{u} = \boldsymbol{j}_{\mathrm{dry}}(x, z) \qquad \nabla \cdot \boldsymbol{j}_{\mathrm{dry}} = 0$$

Atmospheric transport equations

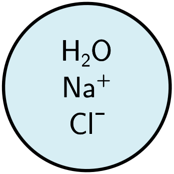
- State variables $\boldsymbol{G} = (\Theta, r_v)$:
  - Dry potential temperature $\quad \Theta = T \left(\dfrac{p^*}{p_{\text{dry}}} \right)^{(\tilde{R}_{\text{dry}}/c_{\text{dry}})}$
  - Water vapor mixing ratio $\quad r_v = \rho_v / \rho_{\text{dry}}$
- Condensation mass density rate ϕ_{con}

Transport equations in the kinematic model

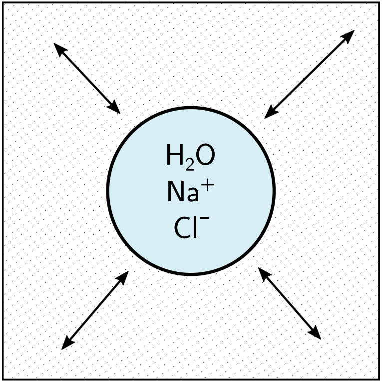
$$\begin{aligned}
\rho_{\text{dry}}\, \partial_t r_v + \nabla \cdot (\rho_{\text{dry}} \boldsymbol{u}\, r_v) &= -\phi_{\text{con}} \\
\rho_{\text{dry}}\, \partial_t \Theta + \nabla \cdot (\rho_{\text{dry}} \boldsymbol{u}\, \Theta) &= \frac{L_v}{c_p\,(1 + \alpha_v\, r_v)} \frac{\Theta}{T}\, \phi_{\text{con}}
\end{aligned}$$

Discrete particle model for cloud droplet

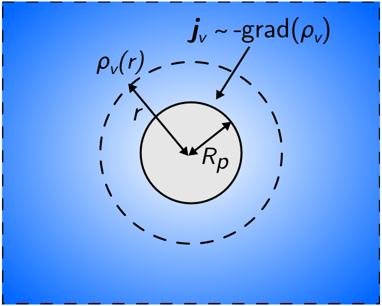
Solution droplet



Fluid-particle interactions?



Mass and heat exchange: Diffusion and conduction



- Diffusion equation for water vapor (source free region $r > R_p$)

$$\frac{\partial \rho_v}{\partial t} + \nabla \cdot \boldsymbol{j}_v = 0$$

$$\boldsymbol{j}_v = -D_v \nabla \rho_v$$

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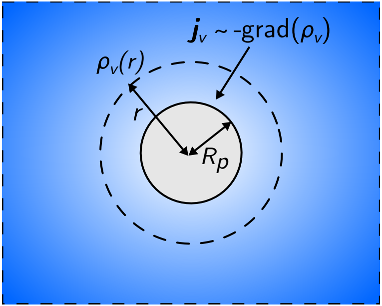

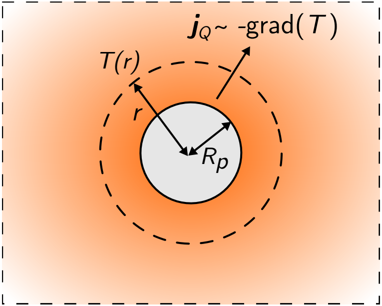

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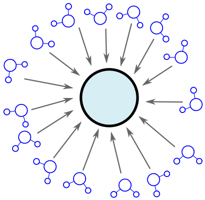
- Heat conduction (source free region $r > R_p$)

$$\rho \, c_p \frac{\partial T}{\partial t} + \nabla \cdot \boldsymbol{j}_Q = 0$$

$$\boldsymbol{j}_Q = -K \nabla T$$

Droplet growth equation



- Latent heat generation = Thermal conduction flow

$$-L_v\,\dot{m} = \dot{Q}$$

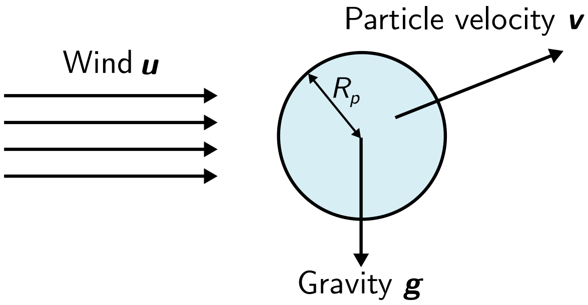
Droplet growth equation

$$\dot{m}_w = 4\pi R_p\, B(R_p, T, p)\,(S - S_{\mathrm{eq}})$$

[Fukuta and Walter (1970), J. Atmos. Sci. **27**, 1160]

- Saturation $S = e/e_s(T)$
- Equilibrium saturation $S_{\mathrm{eq}} = f_{\mathrm{Raoult}}(m_s, m_w)\, f_{\mathrm{Kelvin}}(R_p, T)$

Fluid-particle forces

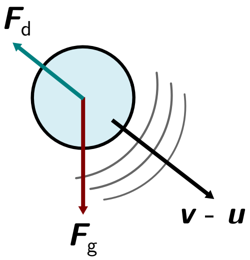


- Relative wind velocity $\tilde{\boldsymbol{u}} = \boldsymbol{u} - \boldsymbol{v}$
- Particle Reynolds number $\mathrm{Re}_p = \dfrac{2\,\rho_f}{\mu_f} R_p |\tilde{\boldsymbol{u}}|$

Modeled particle forces

- Particle Reynolds number $\mathrm{Re}_p = \dfrac{2\,\rho_f}{\mu_f} R_p |\tilde{\boldsymbol{u}}|$
- Drag force + gravity:

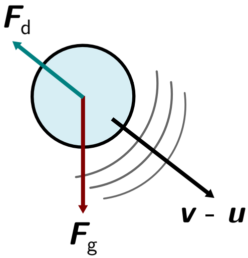
$$\ddot{\boldsymbol{x}} = \frac{\boldsymbol{F}_d + \boldsymbol{F}_g}{m_p} = k_d(R_p, \mathrm{Re}_p)\left[\boldsymbol{u}(\boldsymbol{x}) - \boldsymbol{v}\right] + \boldsymbol{g}$$

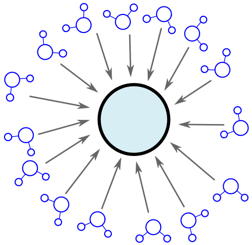


Discrete particle model

Particle equations of motion

$$\dot{\boldsymbol{x}} = \boldsymbol{v}$$
$$\dot{\boldsymbol{v}} = k_d(R_p, \mathrm{Re}_p)\,[\boldsymbol{u} - \boldsymbol{v}] + \boldsymbol{g}$$
$$\dot{m} = 4\pi R_p\, B(R_p)\,[S - S_{\mathrm{eq}}(m)]$$

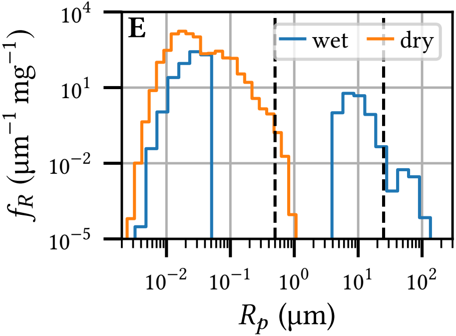




- **Droplet collisions** coming next

Droplet collision-coalescence

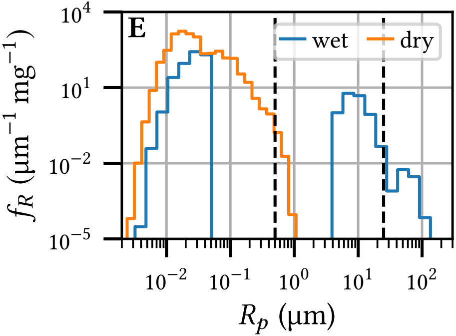
- Droplet size distribution f_R



Droplet collision-coalescence

- Droplet size distribution f_R
- Droplet number concentration

$$\mathrm{DNC}(\boldsymbol{x}, t) = \int \mathrm{d}R\, f_R(R, \boldsymbol{x}, t)$$



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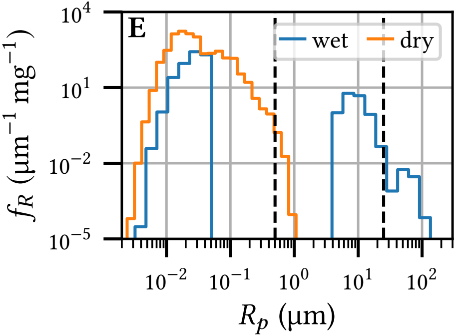

- Mass distribution $f_m = f_R\, \mathrm{d}R/\mathrm{d}m$ with

$$\mathrm{DNC}(\boldsymbol{x}, t) = \int \mathrm{d}m\, f_m(m, \boldsymbol{x}, t)$$

Droplet collision-coalescence

- Coalescence equation

$$\frac{\partial f_m(m,t)}{\partial t} = \frac{1}{2}\int_0^m \mathrm{d}m'\, f_m(m',t)\, f_m(m-m',t)\, K(m',m-m') - \int_0^\infty \mathrm{d}m'\, f_m(m,t)\, f_m(m',t)\, K(m,m')\,.$$

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- Collection kernel

$$K(m,m') := \lim_{\delta t\to 0} \frac{P_{\delta t}(m,m')\,\Delta V}{\delta t}$$

with collection probability $P_{\delta t}(m,m')$

Collision kernels

- Artificial Golovin (sum-of-mass) kernel:

$$K(m, m') = b_G\,(m + m')$$

- Hydrodynamic collection kernel:

$$K(R_1, R_2) = E_c(R_1, R_2)\,\pi\,(R_1 + R_2)^2\,|\boldsymbol{v}_2 - \boldsymbol{v}_1|$$

Super-droplet approach

- Domain: $1500\,\mathrm{m} \times 1\,\mathrm{m} \times 1500\,\mathrm{m}$
- Cloud condensation nuclei (CCN) number concentration = $100\,\mathrm{cm}^{-3}$
- Total number of particles $\sim 1 \times 10^{14} \Rightarrow$ Problem

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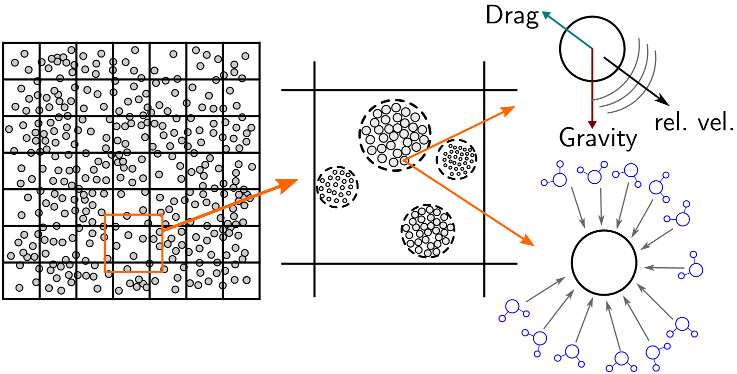
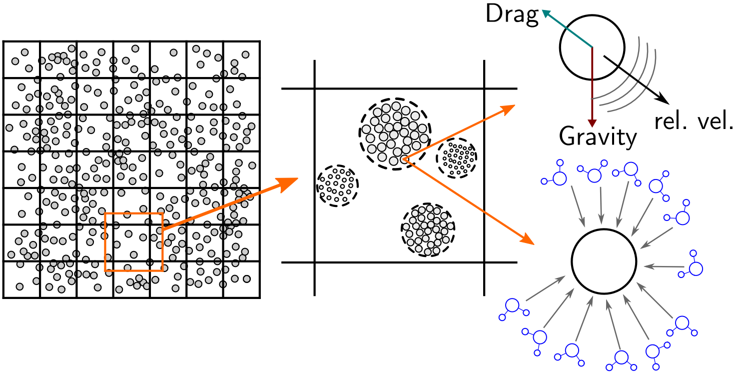
- Super-droplets by [Shima *et al.* (2009), Q. J. R. Meteorol. Soc. **135**, 1307]

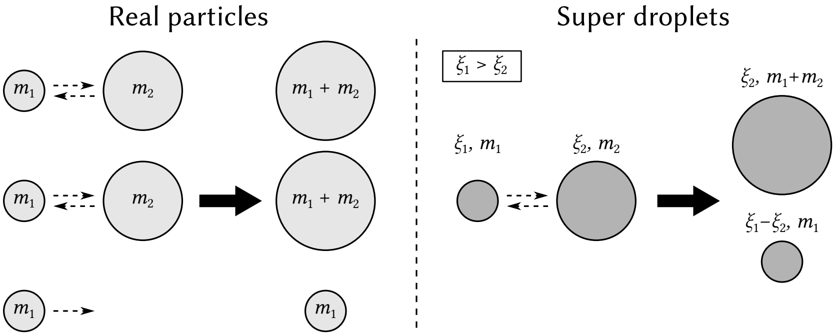


Super-droplet approach

- Super-droplet = Simulation particle (SIP) = Computational particle
- Multiplicity ξ of particles with identical properties
- Equations for (mass m, position $\boldsymbol{x}$, velocity $\boldsymbol{v}$) as before
- Condensation rate in ΔV: $\phi_{\text{con}} = \sum_{\{i\,:\,\boldsymbol{x}_i \in \Delta V\}} \xi_i\, \dot{m}_i / \Delta V$



Super-droplet collisions: All-or-nothing approach



- Coalescence of a super-droplets pair during Δt_{col} with

$$P^{\mathrm{S}}_{\Delta t_{\mathrm{col}}} = \xi_1\, K(R_1, R_2)\, \frac{\Delta t_{\mathrm{col}}}{\Delta V}$$

- Total **average** collision rate $= \xi_1\, \xi_2\, K(R_1, R_2)/\Delta V$

Equations of motion

Particles

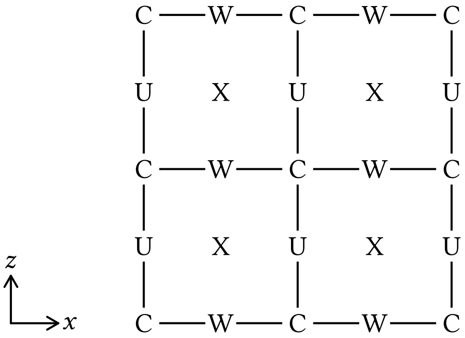
$$\begin{aligned}
\dot{\boldsymbol{x}} &= \boldsymbol{v} \\
\dot{\boldsymbol{v}} &= k_d(R_p, \boldsymbol{v}, \boldsymbol{u}(\boldsymbol{x}))\,[\boldsymbol{u}(\boldsymbol{x}) - \boldsymbol{v}] + \boldsymbol{g} \\
\dot{m} &= 4\pi\, R_p\, B(R_p)\,[S - S_{\mathrm{eq}}]
\end{aligned}$$

Atmospheric advection

$$\begin{aligned}
\rho_{\mathrm{dry}}\,\partial_t r_v + \nabla\cdot(\rho_{\mathrm{dry}}\boldsymbol{u}\, r_v) &= -\phi_{\mathrm{con}} \\
\rho_{\mathrm{dry}}\,\partial_t \Theta + \nabla\cdot(\rho_{\mathrm{dry}}\boldsymbol{u}\,\Theta) &= \frac{L_v}{c_p\,(1+\alpha_v\, r_v)}\,\frac{\Theta}{T}\,\phi_{\mathrm{con}}
\end{aligned}$$

Spatial grid: 2D rectangular Arakawa C-type grid

- Scalar fields (Θ, r_v) at X
- Flow field $\boldsymbol{u} = (u, w)^\top$ at (U, W)



Time integration scheme

- State variables $\boldsymbol{G} = (\Theta, r_v)$
- Equations of motion (short version):

$$\dot{\boldsymbol{x}} = \boldsymbol{v} \qquad \dot{\boldsymbol{v}} = \boldsymbol{a}(\boldsymbol{x}, \boldsymbol{v}, m) \qquad \dot{m} = \gamma(\boldsymbol{x}, m)$$

$$\frac{\mathrm{d}\boldsymbol{G}}{\mathrm{d}t} = \boldsymbol{f}_{\mathrm{adv}}(\boldsymbol{G}) + \boldsymbol{f}_{\mathrm{con}}(\boldsymbol{G}, \phi_{\mathrm{con}})$$

- Time scale separation: **Advection** Δt_{adv}, **collision** Δt_{col} and **condensation** h

Based on [Knoth & Wolke (1998), Appl. Numer. Math. **28**, 327]

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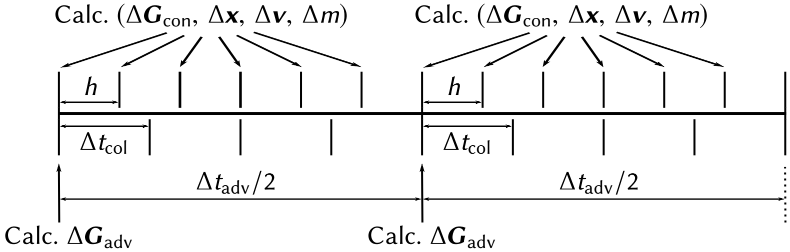


Based on [Knoth & Wolke (1998), Appl. Numer. Math. **28**, 327]

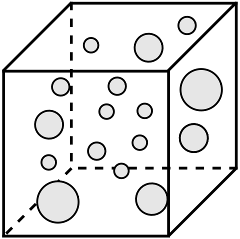
Simulation program

- Program written from scratch during master thesis
- Code in pure Python:
    - Numpy data structure
    - Numba for speed (just-in-time compilation)
    - Parallelization possible, but not implemented
- Available on Github:
  `https://github.com/JanKBohrer/ProgramMasterthesis`

Collision box model

- Particles remain in box ΔV
- Only collisions active
- No condensation/evaporation
- Initial exponential mass distribution

$$f_m(m, t = 0) = \frac{\mathrm{DNC}_0}{\bar{m}_0} \exp\left(-\frac{m}{\bar{m}_0}\right)$$



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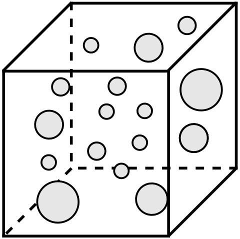


- Logarithmic radius distribution function

$$g_{\ln(R)} := 3\, m^2\, f_m$$

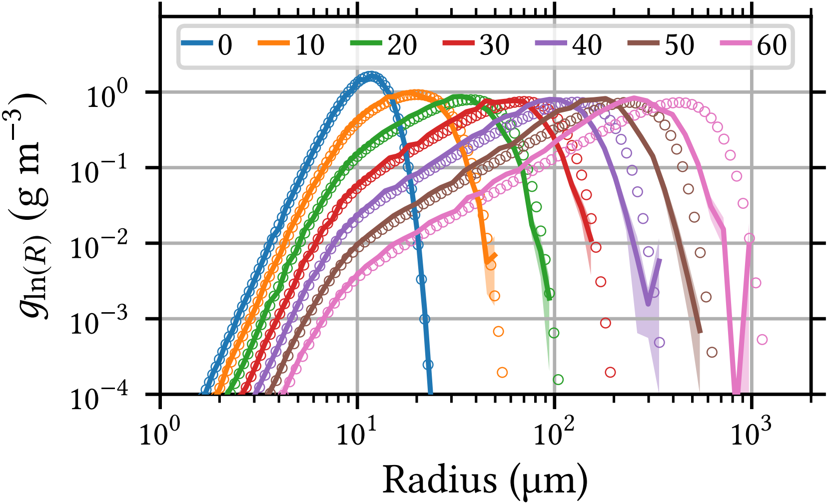
- Liquid mass content (total mass per volume)

$$\mathrm{LMC} = \int \mathrm{d}(\ln R)\, g_{\ln(R)}(R)$$

Evolution of the size distribution (Golovin collision kernel)

- 50 super-droplets per cell, average over 500 simulation runs

Analytic reference (circles), Legend: Time in minutes



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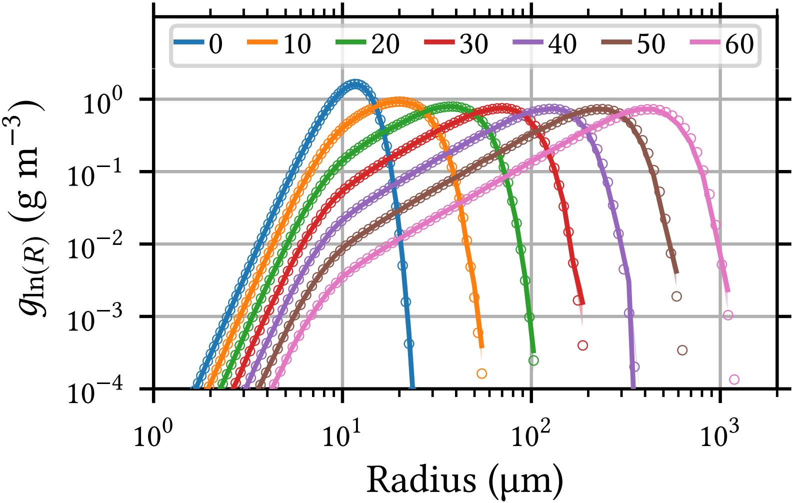
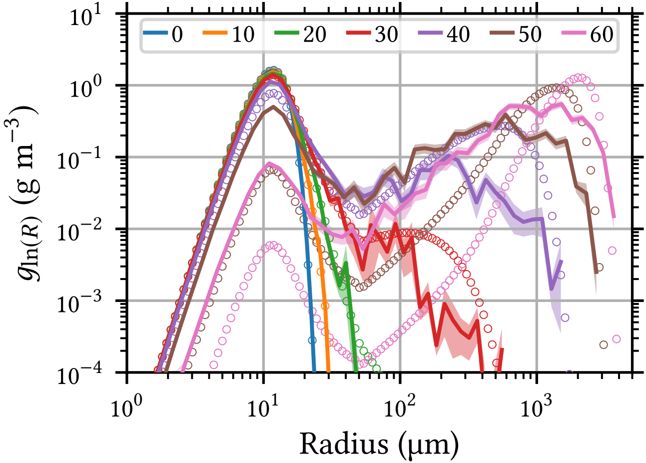


Evolution of the size distribution (Long collision kernel)

- 50 super-droplets per cell, average over 500 simulation runs
- Bin model reference: [Wang, Xue & Grabowski (2007), J. Comp. Phys. **226**, 59]

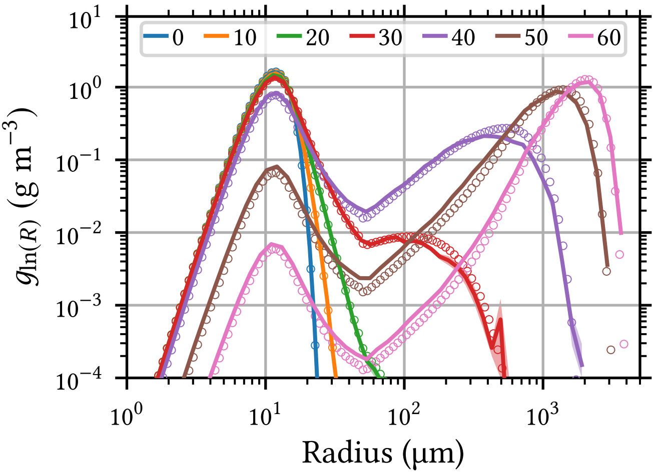
Bin model reference (circles), Legend: Time in minutes



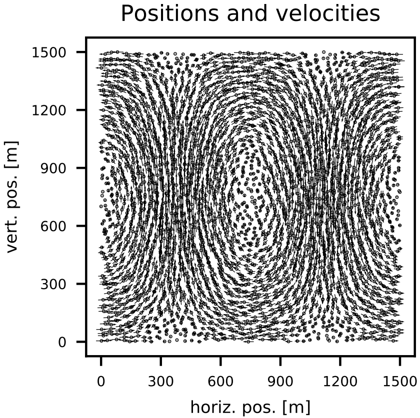
Evolution of the size distribution (Long collision kernel)

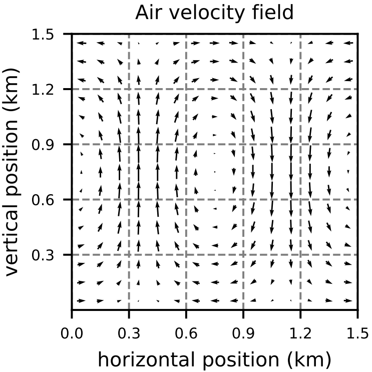
- 15 000 super-droplets per cell, average over 500 simulation runs
- Bin model reference: [Wang, Xue & Grabowski (2007), J. Comp. Phys. **226**, 59]

Bin model reference (circles), Legend: Time in minutes



Particle initialization

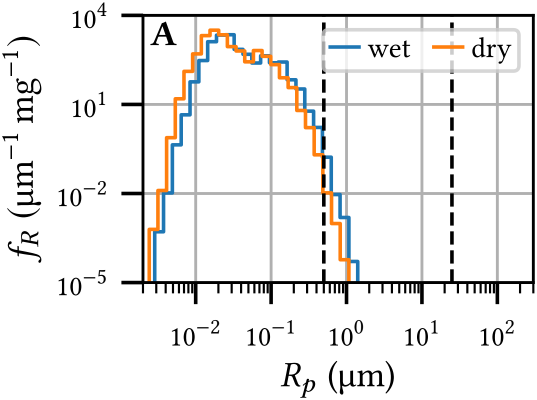




Particle dry size distribution

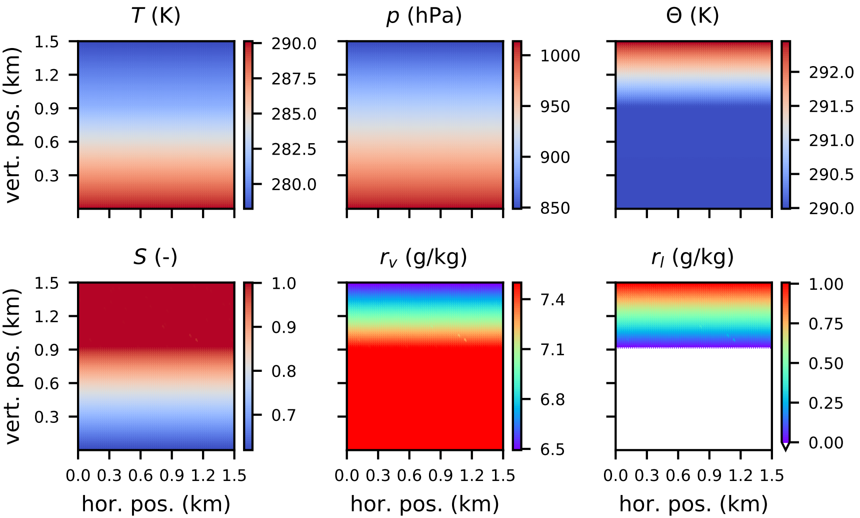
- Bimodal log-normal distribution [Allen *et al.* (2011), Atmos. Chem. Phys. **11**, 5237]

$$f_{R,s}(R_s) = \sum_{k=1}^{2} \frac{\mathrm{DNC}_k}{\sqrt{2\pi}\,\ln\left(\sigma^*_{R,k}\right) R_s} \exp\left[-\left(\frac{\ln\left(R_s/\mu^*_{R,k}\right)}{\sqrt{2}\,\ln\left(\sigma^*_{R,k}\right)}\right)^2\right]$$



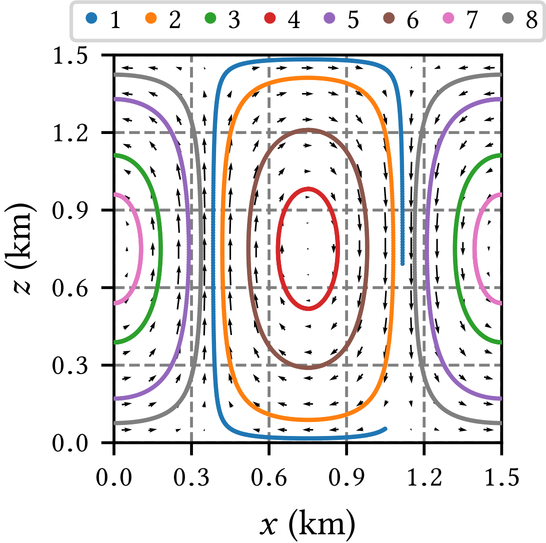
Atmospheric 2D kinematic model: Initialization

- Conditions: Θ_{liquid} = const. = 289 K, $r_{\text{tot}} = r_v + r_l$ = const. = 7.5 g/kg



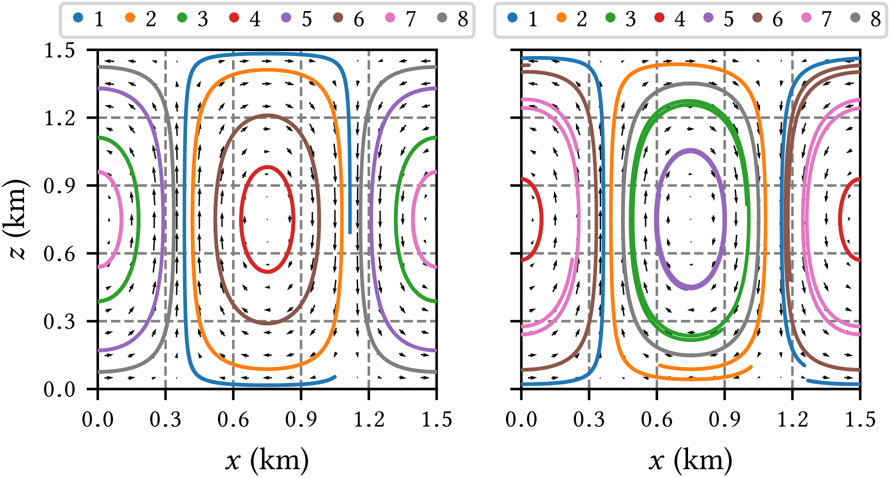
Particle trajectories

- Spin-up phase: No gravity, no collisions

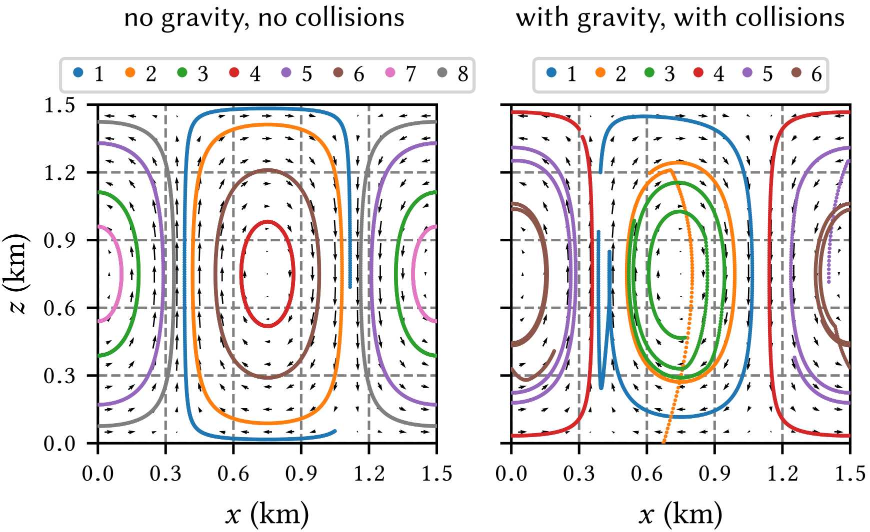


Particle trajectories

no gravity, no collisions | with gravity, no collisions



Particle trajectories

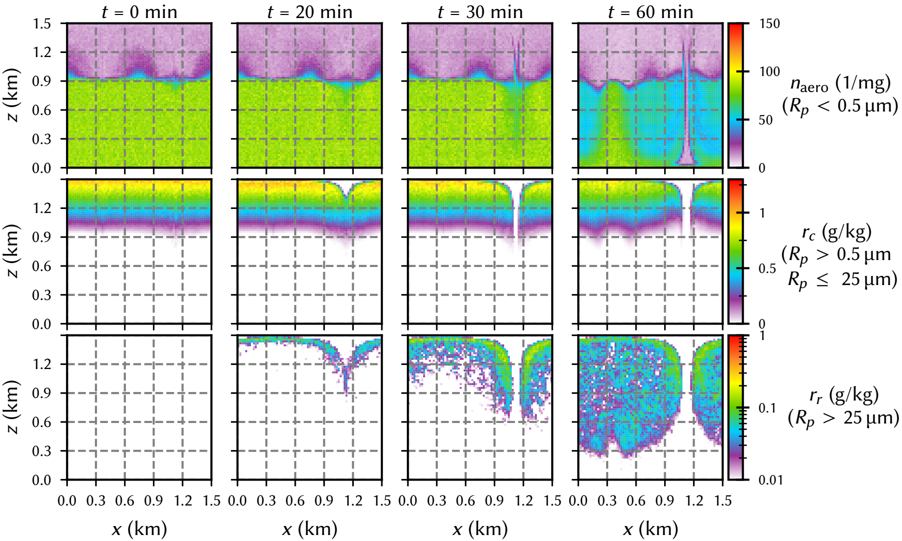


Default parameters

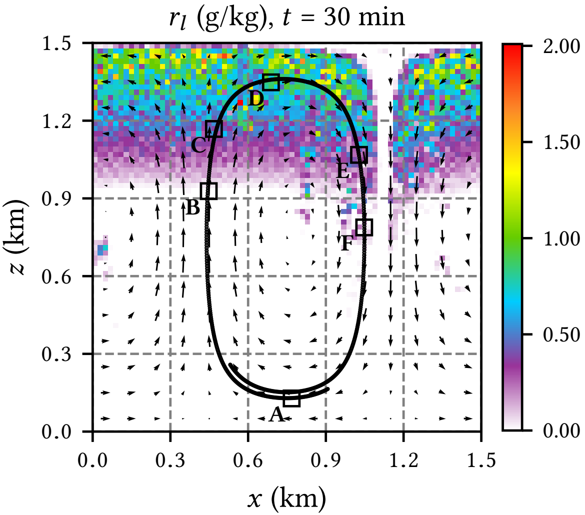
- CCN material: Ammonium sulfate
- $\mathrm{DNC}_1 + \mathrm{DNC}_2 = 60\,\mathrm{cm}^{-3} + 40\,\mathrm{cm}^{-3} = 100\,\mathrm{cm}^{-3}$
- 64 super-droplets per cell
- 75×75 grid cells of $20\,\mathrm{m} \times 20\,\mathrm{m}$
- Time steps: $\Delta t_{\mathrm{adv}} = 1\,\mathrm{s}, \quad \Delta t_{\mathrm{col}} = 0.5\,\mathrm{s}, \quad h = 0.1\,\mathrm{s}$
- Hydrodynamic Long collision kernel
- 2 hour spin-up phase
- **Results are averages** over 50 independent simulations

Test case: Cloud evolution

- Ammonium sulfate CCNs, Long kernel, average over 50 simulation runs

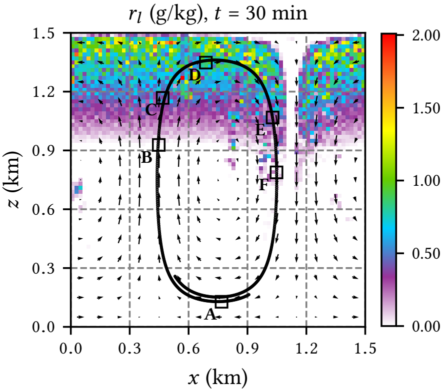


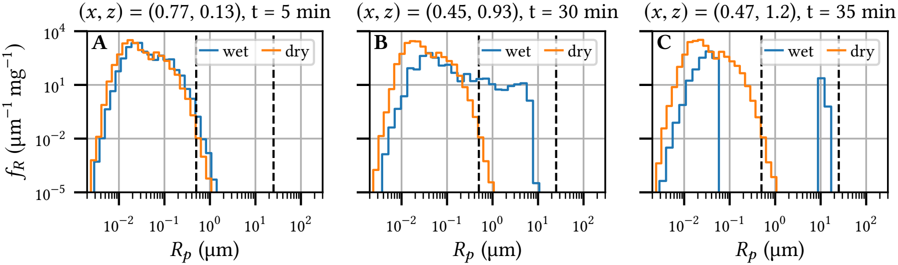
Droplet growth cycle



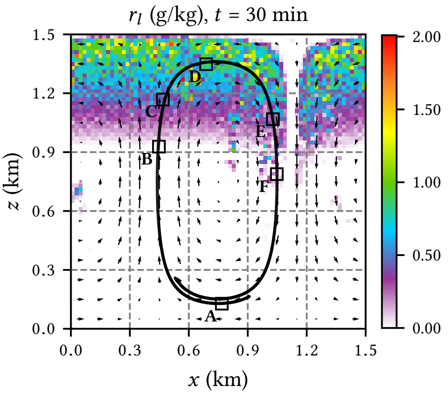
t (min): **A**: 5, **B**: 30, **C**: 35, **D**: 45, **E**: 60, **F**: 65

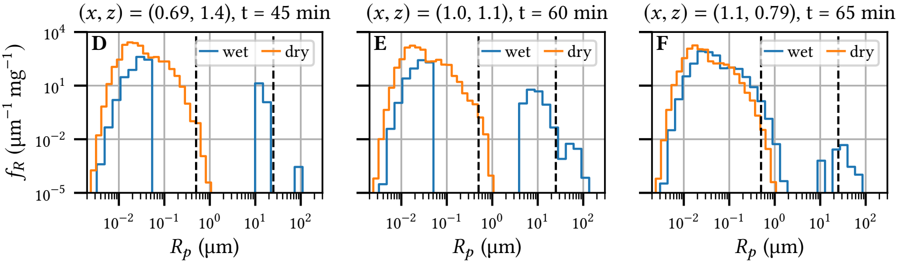
Droplet growth cycle





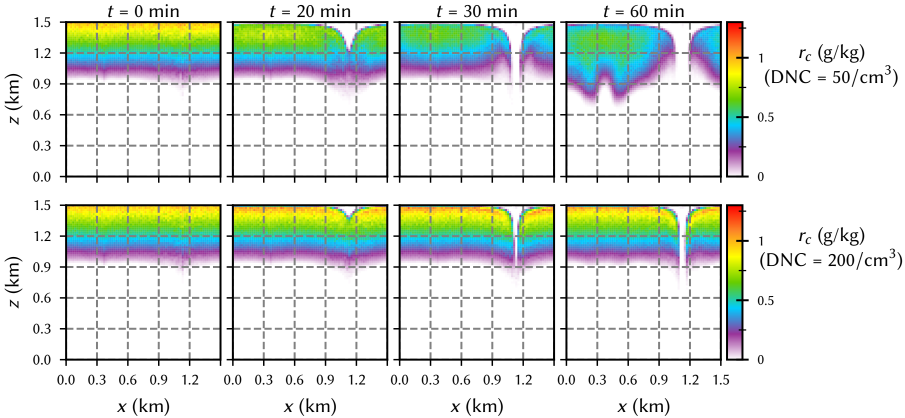
Droplet growth cycle





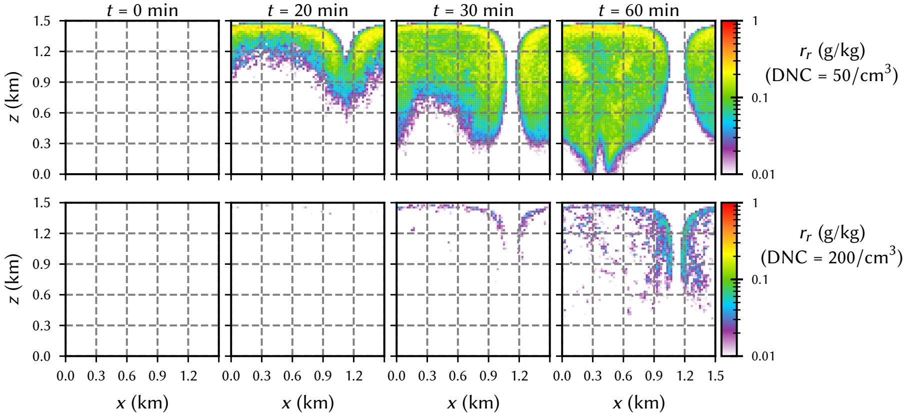
Variation of the CCN number concentration

- Cloud water mixing ratio r_c $\quad (0.5\,\mu\text{m} < R_p \leq 25\,\mu\text{m})$



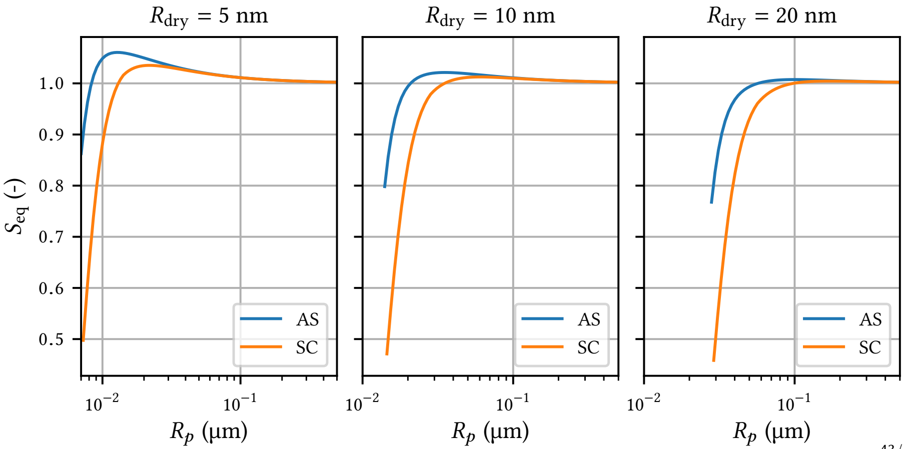
Variation of the CCN number concentration

- Rain water mixing ratio r_r $\quad (R_p > 25\,\mu m)$



Variation of CCN material

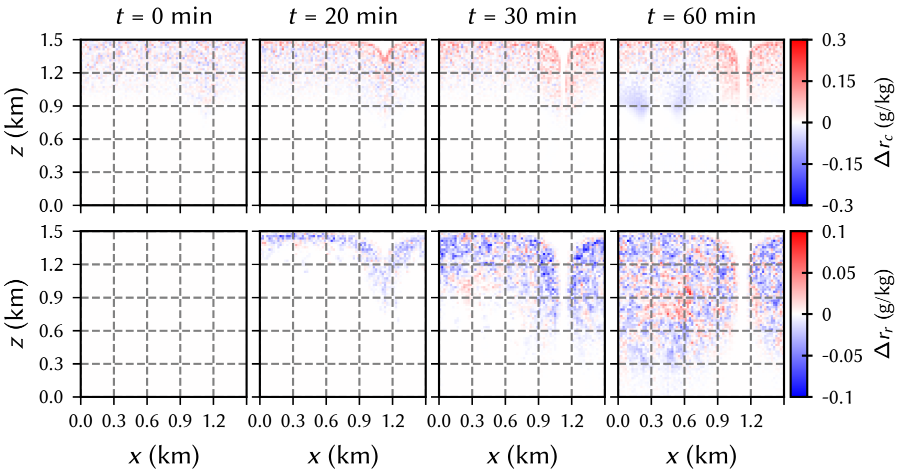
- Equilibrium saturations for
  - **Ammonium sulfate** (AS, blue)
  - **Sodium chloride** (SC, orange)



Variation of CCN material

- Difference for **sodium chloride** (SC) and **ammonium sulfate** (AS):

$$\Delta r = r_{SC} - r_{AS}$$



Conclusions

- Stable, extendable program
- Agreement of collision box model simulations with most recent results of [Unterstrasser, Hoffmann & Lerch (2017), Geosci. Model Dev. **10**, 1521]
- Results of 2D test case comparable to [Arabas *et al.* (2015), Geosci. Model Dev. **8**, 1677]
- Plausible behavior when varying CCN concentration and material

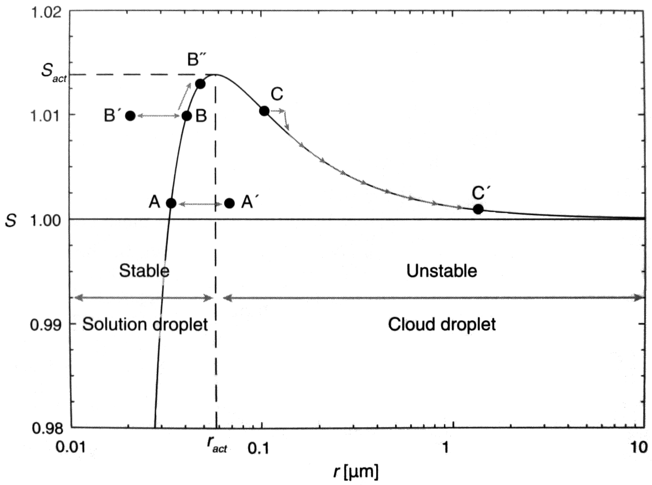
Outlook: Possible extensions

- Parallelization for speed
- 3D model coupled to computational fluid dynamics solver
  - see e.g. [Pressel *et al.* (2015), J. Adv. Model. Earth Sy. **7**, 1425]
- Multicomponent chemistry
  - see e.g. [Jaruga & Pawlowska (2018) Geosci. Model Dev. **11**, 3623]
- Ice crystal systems
  - see e.g. [Sölch & Kärcher (2010), Q. J. R. Meteorol. Soc. **136**, 2074]
- Local turbulence treatment by stochastic velocity perturbations
  - see e.g. [Grabowski & Abade (2017), J. Atmos. Sci. **74**, 1485]

Thank you for your attention!

Any questions?

Equilibrium saturation: Köhler curve



Lohmann, Lüönd, Mahrt: *An introduction to clouds*, Cambridge Univ. Press 2016

$$S_{\mathrm{eq}} = \frac{e_s(T, R_p, m_s)}{e_s(T, R_p = \infty, m_s = 0)} = \frac{m_w}{m_w + m_s\, i_s\, M_w/M_s} \exp\left(\frac{a_{\mathrm{K}}}{R_p}\right)$$