Discrete particle methods for a scalable atmospheric dynamics solver

Jan Bohrer[1], Oswald Knoth[1]

1 Leibniz Institute for Tropospheric Research, Leipzig, Germany

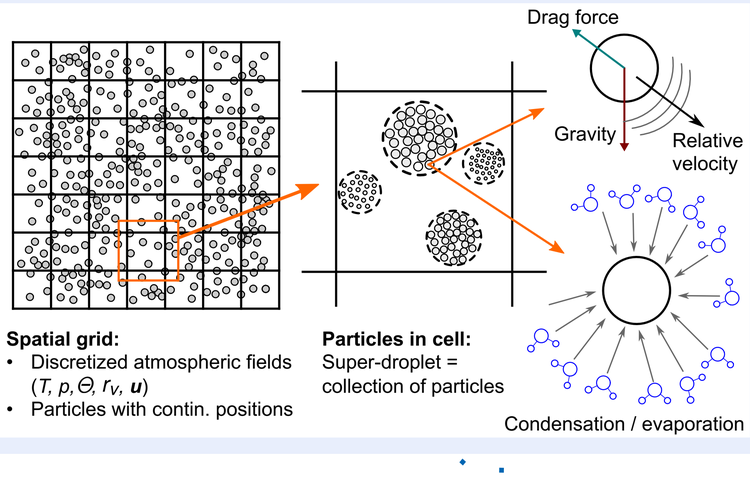
bohrer@tropos.de

TROPOS
Leibniz Institute for Tropospheric Research

Leibniz Association

Introduction

We aim to extend an existing scalable solver for atmospheric applications (All Scale Atmospheric Model, ASAM) by a two-way coupled Euler-Lagrangian model for the description of cloud processes on a broad range of dimensional scales. By coupling Computational Fluid Dynamics (CFD) and Discrete Particle Methods (DPM) it is possible to obtain a sophisticated representation of the dynamical movement and continuous mass evolution of the droplets. While the surrounding moist air is described as continuous fluid, the aqueous solution cloud droplets are considered to be discrete particles of finite size, which interact with the carrier fluid phase by momentum, mass and heat exchange. The distinct particle approach enables a detailed generation and analysis of droplet size distributions. Moreover, the sedimentation as well as the collision and break-up can be modeled close to natural processes. Since the number of cloud particles in atmospheric domains exceeds computational limitations by orders of magnitudes, we use the super-droplet model proposed by [Shi09], where one computational particle represents a collection of particles with identical physical properties.



Spatial grid:
- Discretized atmospheric fields (T, p, Θ, r_v, $\boldsymbol{u}$)
- Particles with contin. positions

Particles in cell:
Super-droplet = collection of particles

Model

Cloud droplet model

Droplets are treated as rigid spherical particles with variable radius R_p and mass m_p and may contain water (w) as well as insoluble and soluble species (s), such as cloud condensation nuclei (CCN). One computational "super-droplet" represents a multiplicity ξ of droplets with identical physical properties (position, mass, velocity, …) [Shi09].

The total force acting on a particle moving with velocity $\boldsymbol{v}$ through air with local velocity $\boldsymbol{u}$ is modeled by the sum of drag force and gravity:

$$m_p \ddot{\boldsymbol{x}}_p = \boldsymbol{F}_d + \boldsymbol{F}_g = m_p k_d (\boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{v}) + m_p \boldsymbol{g} ,$$

where the drag parameter $k_d(\mathrm{Re}_p)$ depends on the regime of the particle Reynolds number $\mathrm{Re}_p = 2\rho_f R_p |\boldsymbol{u} - \boldsymbol{v}| / \mu_f$ [Zhu07].

Each droplet exchanges water with the surrounding moist air due to condensation and evaporation with mass rate [Fuk70]

$$\dot{m}_w =: \gamma = R_p \left(S(r_v, T) - S_{\mathrm{eq}}\right) B\left(R_p, T, p\right) ,$$

where $S = R_v \rho_{\mathrm{dry}} r_v T / e_{\mathrm{sat}}(T)$ is the ambient saturation, $r_v = \rho_v / \rho_{\mathrm{dry}}$ the water vapor mixing ratio, e_{sat} the saturation pressure and B a kinetic term. The equilibrium saturation is given by Köhler theory as

$$S_{\mathrm{eq}} = \frac{m_w}{m_w + \sum_s m_s i_s M_w / M_s} \exp\left(\frac{2\sigma_w}{R_v T \rho_p R_p}\right) .$$

Advection with condensation source term

The fluid velocity $\boldsymbol{u}(\boldsymbol{x}, t)$ is either stationary or simultaneously calculated by a CFD solver. Water vapor ($\rho_{\mathrm{dry}} r_v$) and thermal energy ($\rho_{\mathrm{dry}} \Theta$) are exchanged by condensation with rate ϕ_{cond} (source term) and transported by atmospheric advection:

$$\partial_t(\rho_{\mathrm{dry}}\, r_v) = -\nabla \cdot (\rho_{\mathrm{dry}}\, r_v\, \boldsymbol{u}) - \phi_{\mathrm{cond}}$$
$$\partial_t(\rho_{\mathrm{dry}}\, \Theta) = -\nabla \cdot (\rho_{\mathrm{dry}}\, \Theta\, \boldsymbol{u}) + \frac{L_v\, \Theta}{c_{p,\mathrm{dry}}\, T} \phi_{\mathrm{cond}}$$

Time integration

Equations of motion

The fluid state variables $\boldsymbol{G} := (\Theta, r_v)^\top$ are discretized on a rectangular spatial grid. Their time evolution consists of an advection and a condensation part:

$$\dot{\boldsymbol{G}} = \boldsymbol{f}_{\mathrm{ad}}(\boldsymbol{G}) + \boldsymbol{f}_{\mathrm{cond}}(\boldsymbol{G}, \phi_{\mathrm{cond}})$$

The equations for particle position, velocity and water mass are given by

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

Timescale separation

We separate the dynamics in "slow" atmospheric advection with time step Δt_{ad} and "fast" particle interactions with time step $h = \Delta t_{\mathrm{ad}}/N$, such that the discrete time may be described by

$$t_n^k = n\,\Delta t_{\mathrm{ad}} + k\,h \quad \Rightarrow \quad t_n^{k+N} = t_{n+1}^k .$$

Source free advection

Without any sources, a second order Runge-Kutta scheme is formulated as

$$\boldsymbol{G}_{n+1/2} = \boldsymbol{G}_n^{N/2} = \boldsymbol{G}_n + \Delta t_{\mathrm{ad}} \boldsymbol{f}_{\mathrm{ad}}(\boldsymbol{G}_n)/2$$
$$\boldsymbol{G}_{n+1} = \boldsymbol{G}_n^{N} = \boldsymbol{G}_n + \Delta t_{\mathrm{ad}} \boldsymbol{f}_{\mathrm{ad}}(\boldsymbol{G}_{n+1/2})$$
$$\Rightarrow \Delta \boldsymbol{G}_n = \boldsymbol{G}_{n+1} - \boldsymbol{G}_n = \Delta t_{\mathrm{ad}} \boldsymbol{f}_{\mathrm{ad}}\left(\boldsymbol{G}_n^{N/2}\right) .$$

Subloop integration scheme

The particle interactions are integrated in a subloop $t_n^0 \le t < t_{n+1}^0$. We use the midpoint rule for the particle positions and purely implicit methods for velocities and masses.

Assuming the fluid field $\boldsymbol{u}(\boldsymbol{x}, t)$ is known, the following scheme describes the evolution of state variables and all particles in any given grid cell during one sub step $t \to t + h$:

$$\boldsymbol{x}_*^k = \boldsymbol{x}^k + \frac{h}{2}\boldsymbol{v}^k$$
$$m^{k+1} = m^k + h\gamma\left(\boldsymbol{x}_*^k, m^{k+1}, t^{k+1}\right)$$
$$\boldsymbol{v}^{k+1} = \boldsymbol{v}^k + h\boldsymbol{a}\left(\boldsymbol{x}_*^k, \boldsymbol{v}^{k+1}, m^{k+1}, t^{k+1}\right)$$
$$\boldsymbol{x}^{k+1} = \boldsymbol{x}_*^k + \frac{h}{2}\boldsymbol{v}^{k+1}$$
$$\boldsymbol{G}^{k+1} = \boldsymbol{G}^k + \Delta \boldsymbol{G}_{\mathrm{ad}}^k + \boldsymbol{f}_{\mathrm{cond}}(\boldsymbol{G}^k, \phi_{\mathrm{cond}}^k)$$

The condensation rate is averaged over time and grid cell volume V_0:

$$\phi_{\mathrm{cond}}^k = \sum_{\alpha \in \mathrm{cell}} \frac{\Delta m_\alpha^k}{V_0\, h}$$

The change by advection is spread over the subloop using a modified Runge-Kutta method (cf. source free advection):

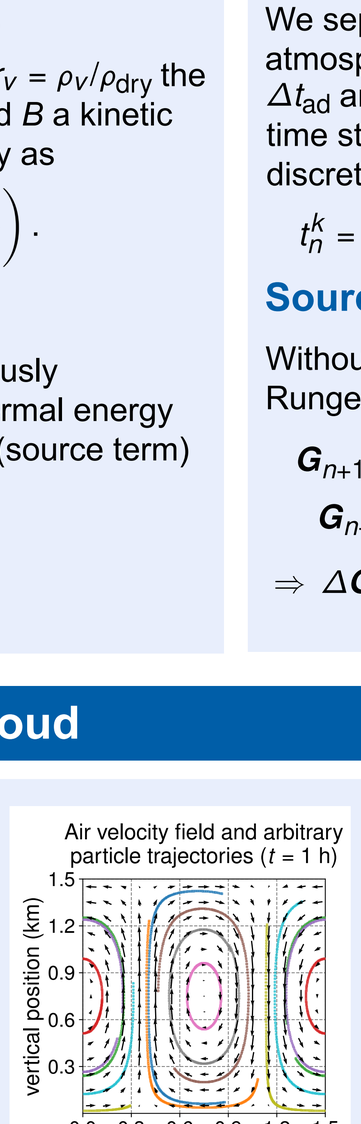
$$\Delta \boldsymbol{G}_{\mathrm{ad}}^k = \begin{cases} \boldsymbol{f}_{\mathrm{ad}}\left(\boldsymbol{G}^0\right), & 0 \le k < \frac{N}{2} \\ 2\,\boldsymbol{f}_{\mathrm{ad}}\left(\boldsymbol{G}^{N/2}\right) - \boldsymbol{f}_{\mathrm{ad}}\left(\boldsymbol{G}^0\right), & \frac{N}{2} \le k < N \end{cases}$$

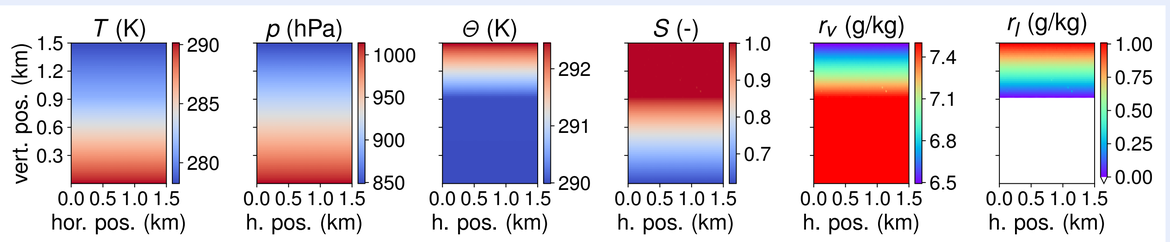
Test case: Drizzling stratocumulus cloud

We use a 2D kinematic framework ([Muh13], case 1) with periodic boundary conditions, stationary dry air density profile and velocity field $\rho_{\mathrm{dry}}\boldsymbol{u} = \nabla \times (\psi(x, z)\hat{\boldsymbol{e}}_y)$ defined by the stream function [Ras11]

$$\psi(x, z) = -J_{\max} X/\pi \sin(\pi z / Z) \cos(2\pi x / X) .$$

Starting from a hydrostatic atmosphere, the total water content is decomposed into water vapor and liquid water by saturation adjustment with boundary conditions $r_{\mathrm{tot}} = r_v + r_l = 7.5\,\mathrm{g/kg}$ and $\Theta_{\mathrm{liq}} = 289\,\mathrm{K}$.



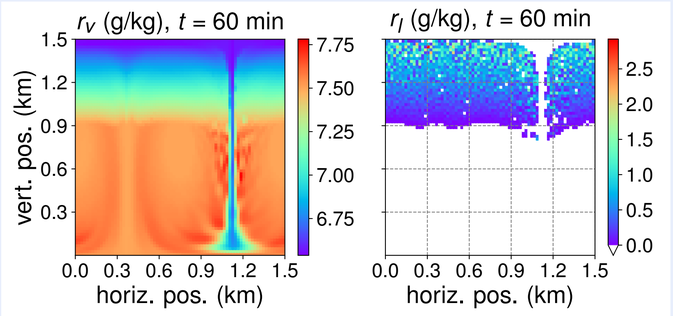


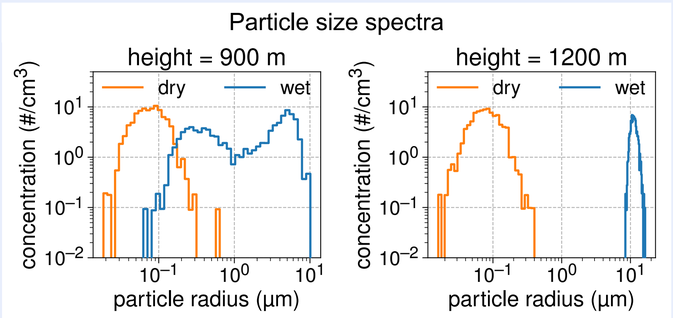
Simulation results

We present results of a one hour simulation run with monomodal dry size spectrum of NaCl CCN (initial total conc. of $100\,\mathrm{cm}^{-3}$). The grid consists of 75 x 75 cells and includes 22500 super-droplets in total ($\xi \sim 1 \times 10^{10}$).

Gravitation leads to a deviation of the trajectories from circular paths for heavy, wet particles and thereby to the formation of downdraft tunnels for r_l and r_v.

For this monomodal case, all droplets get activated and the wet size distribution inside the cloud shows a narrow peak.





Outlook

- Implement model for collision and break-up of droplets
- Extend for multi-component solutions and ice crystal systems
- Investigate turbulence effects and the importance of disregarded interactions
- Extend to 3D and couple to ASAM CFD solver

References

[Fuk70] Fukuta, N.; Walter, L. A. *J. Atmos. Sci.* 1970, **27**, 1160.
[Muh13] Muhlbauer, A.; and Coauthors. *Bull. Am. Meteorol. Soc.* 2013, **94**(5), 45.
[Ras11] Rasinski, P.; Pawlowska, H.; Grabowski, W. W. *Atmos. Res.* 2011, **102**, 120.
[Shi09] Shima, S.; Kusano, K.; Kawano, A.; Sugiyama, T.; Kawahara, S. *Q. J. Royal Meteorol. Soc.* 2009, **135**, 1307.
[Zhu07] Zhu, H. P.; Zhou, Z. Y.; Yang, R. Y.; Yu, A. B. *Chem. Eng. Sci.* 2007, **62**(13), 3378.