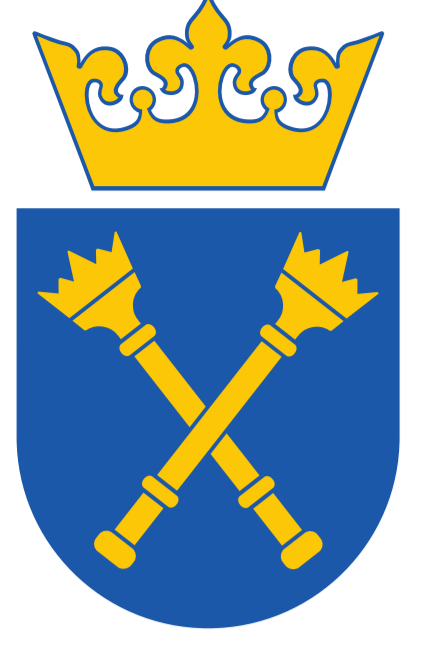


# On Numerical Broadening of Droplet-Size Spectra

**Abstract.** This work discusses the numerical aspects of representing the condensational growth of particles in models of aerosol systems such as atmospheric clouds. It focuses on the Eulerian modelling approach, in which fixed-bin discretisation is used for the probability density function describing the particle-size spectrum. Numerical diffusion is inherent to the employment of the fixed-bin discretisation for solving the arising transport problem (advection equation describing size spectrum evolution). The focus of this work is on a technique for reducing the numerical diffusion based on the upwind scheme: the multidimensional advection algorithm (MPDATA). Several MPDATA variants are explored including infinite-gauge, non-oscillatory, third-order terms and recursive anti-diffusive correction (double-pass donor cell, DPDC) options. Methodologies for handling coordinate transformations associated with numerical grid layout for different discretisations and with the performance of the scheme for different test case parameters and different settings of the algorithm are analysed using (i) an analytically solvable box-model test case formed using (i) an analytically solvable box-model test case and (ii) the single-column kinematic driver (“KiD”) test case in which the size-spectral advection due to condensation is solved simultaneously with the advection in the vertical spatial coordinate, and in which the supersaturation evolution is coupled with the droplet growth through water mass budget. The box-model problem covers size-spectral dynamics only; no spatial dimension is considered. The single-column test case involves a numerical solution of a two-dimensional advection problem (spectral and spatial dimensions). The discussion presented in the paper covers size-spectral, spatial and temporal convergence as well as computational cost, conservativeness and quantification of the numerical broadening of the particle-size spectrum. The box-model simulations demonstrate that, compared with upwind solutions, even a 10-fold decrease in the spurious numerical spectral broadening can be obtained by an apt choice of the MPDATA variant (maintaining the same spatial and temporal resolution), yet at an increased computational cost. Analyses using the single-column test case reveal that the width of the droplet size spectrum is affected by numerical diffusion pertinent to both spatial and spectral advection. Application of even a single corrective iteration of MPDATA robustly decreases the relative dispersion of the droplet spectrum, roughly by a factor of 2 at the levels of maximal liquid water content. Presented simulations are carried out using PyMPDATA – a new open-source Python implementation of MPDATA based on the Numba just-in-time compilation infrastructure.

Sylwester Arabas, Michael Olesik, Jakub Banaśkiewicz, Piotr Bartman, Simon Unterstrasser & Manuel Baumgartner



JAGIELLONIAN UNIVERSITY  
IN KRAKÓW



DLR



JOHANNES GUTENBERG  
UNIVERSITÄT MAINZ

## MPDATA (Smolarkiewicz 1983, ...):

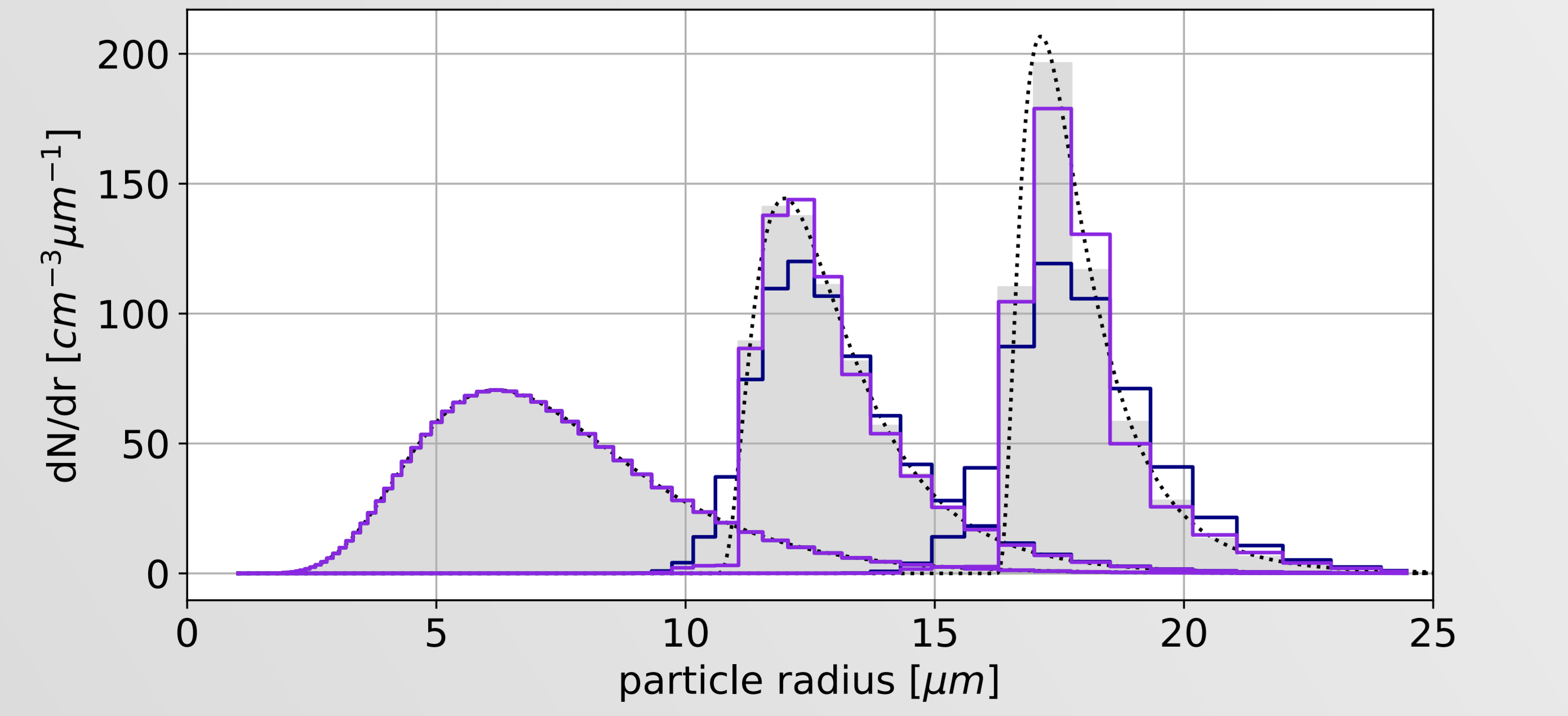
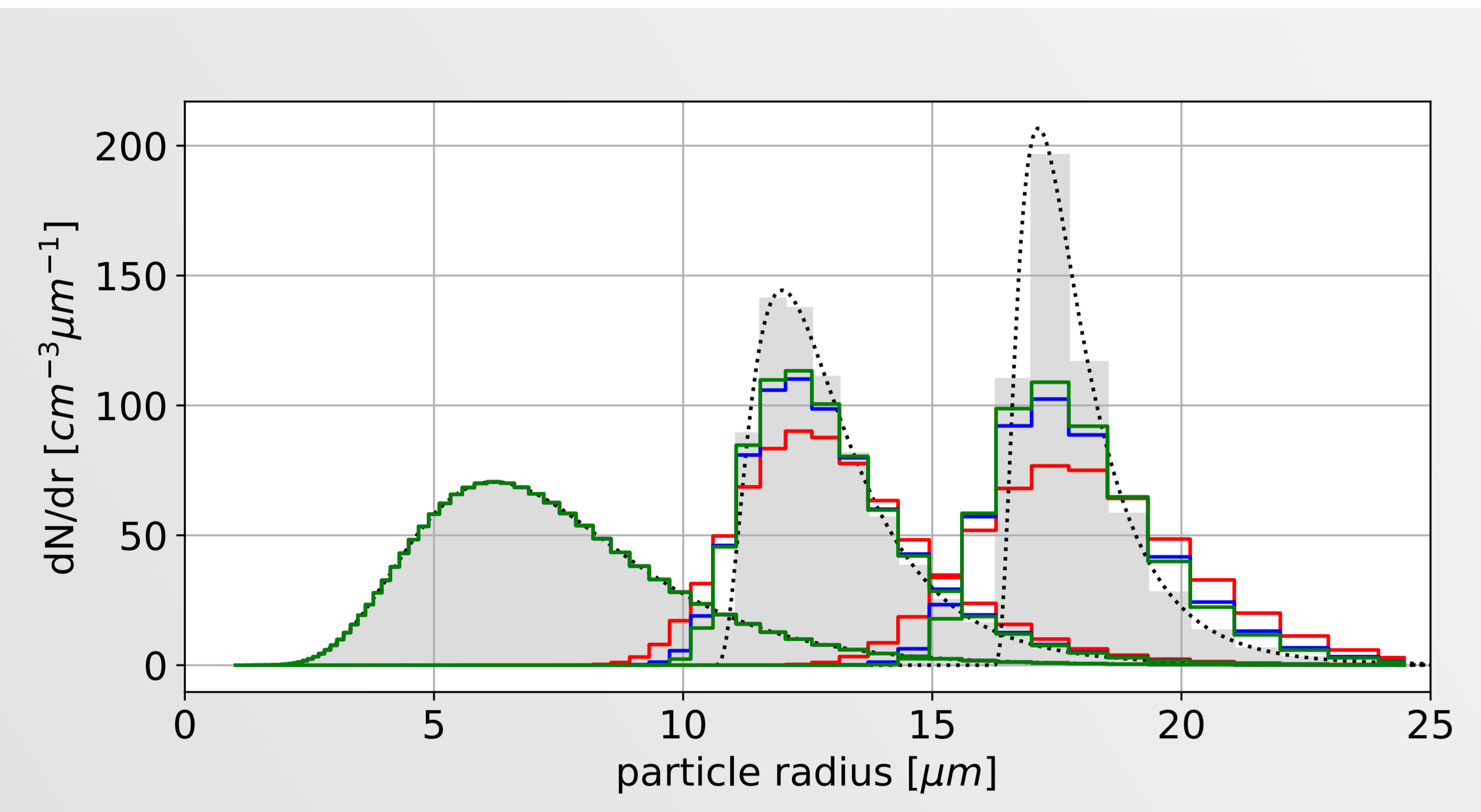
- upwind-based advection scheme with corrective iterations reducing numerical diffusion
- numerous variants developed over the years
- applicable for bin-microphysics transport (both spatial and spectral advection)

## take-home messages from this study:

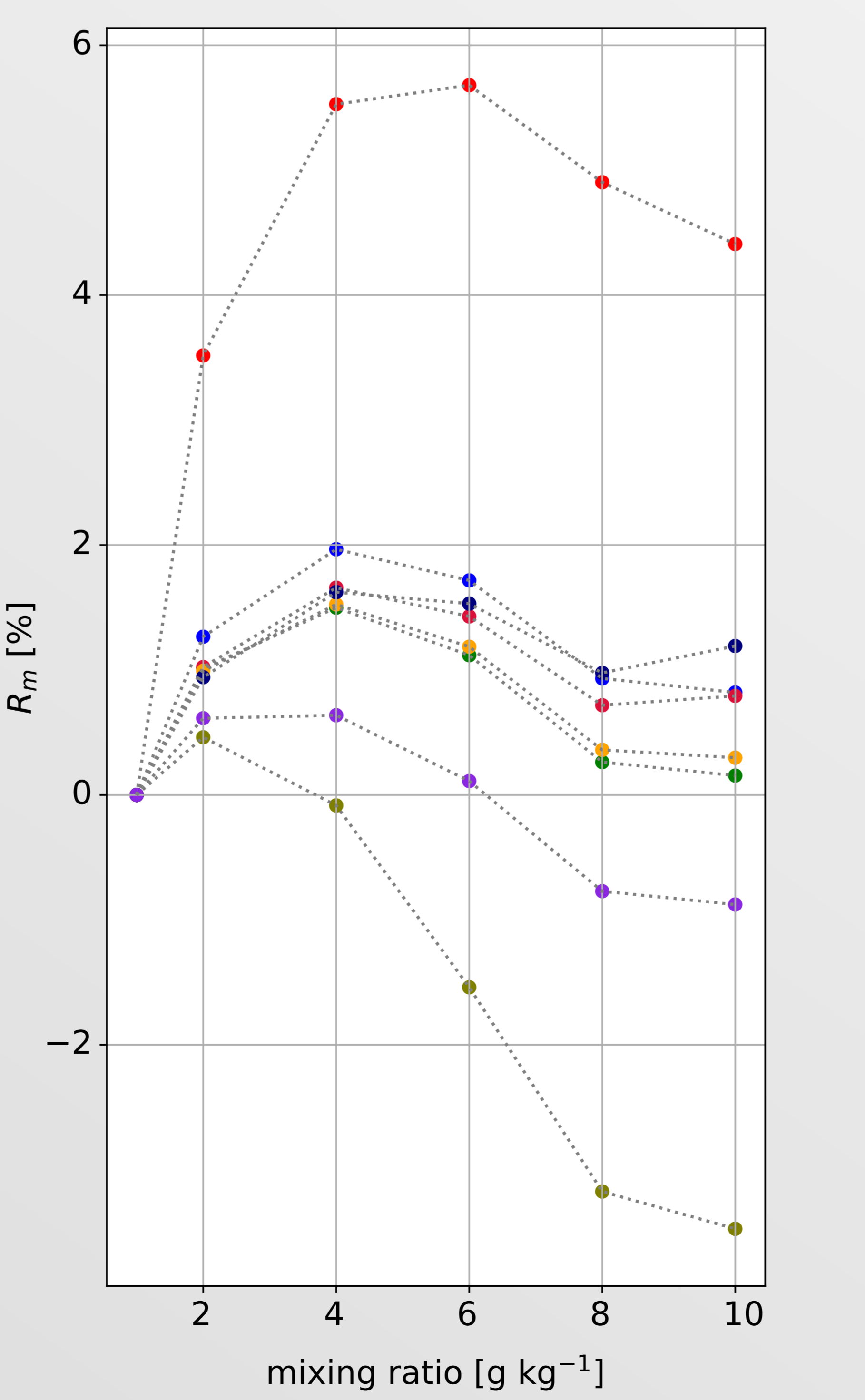
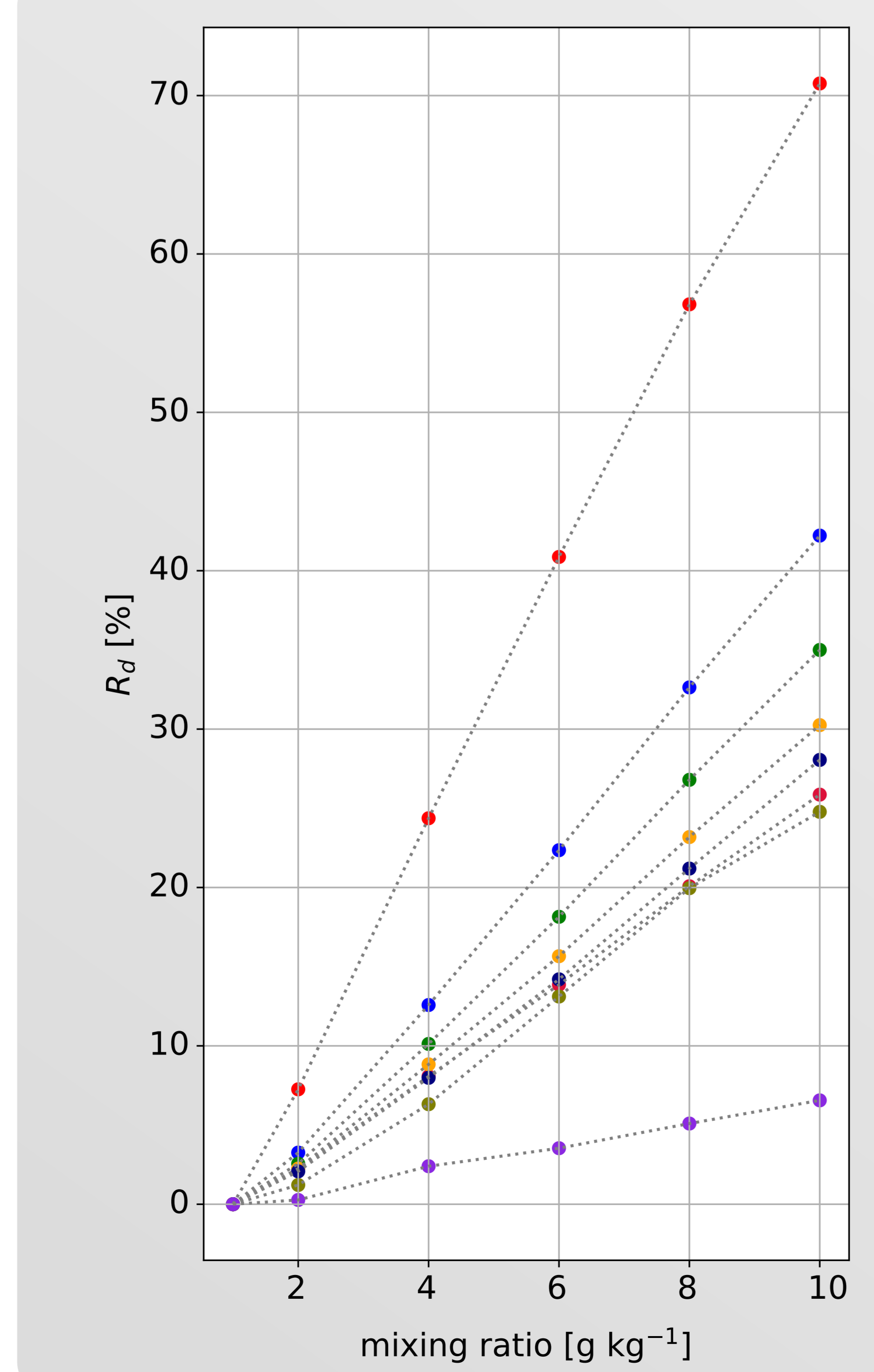
- MPDATA variant choice of great importance (see figure below with  $R_d$ : ratio of numerical to analytical relative dispersion minus one;  $R_m$ : ratio of num. to analyt. water mass -1)
- spatio-spectral advection solution detailed (incl. coupling with supersaturation field within MPDATA corrective iterations)
- all simulations carried out using PyMPDATA: new pure-Python (Numba) MPDATA package



KiD (single-column)  
spatio-spectral advection



box-model setup  
spectral advection only



- upwind
- MPDATA 2 iterations
- MPDATA 3 iterations
- MPDATA 2 iterations infinite gauge
- MPDATA 2 iterations infinite gauge non-oscillatory
- MPDATA 2 iterations DPDC infinite gauge non-oscillatory
- MPDATA 3 iterations third order terms
- MPDATA 3 iterations third order terms infinite gauge non-oscillatory

