Handling particle complexity for simulation of aerosol indirect effects in large scale models

Objective: Efficient aerosol simulation using quadrature-based approaches

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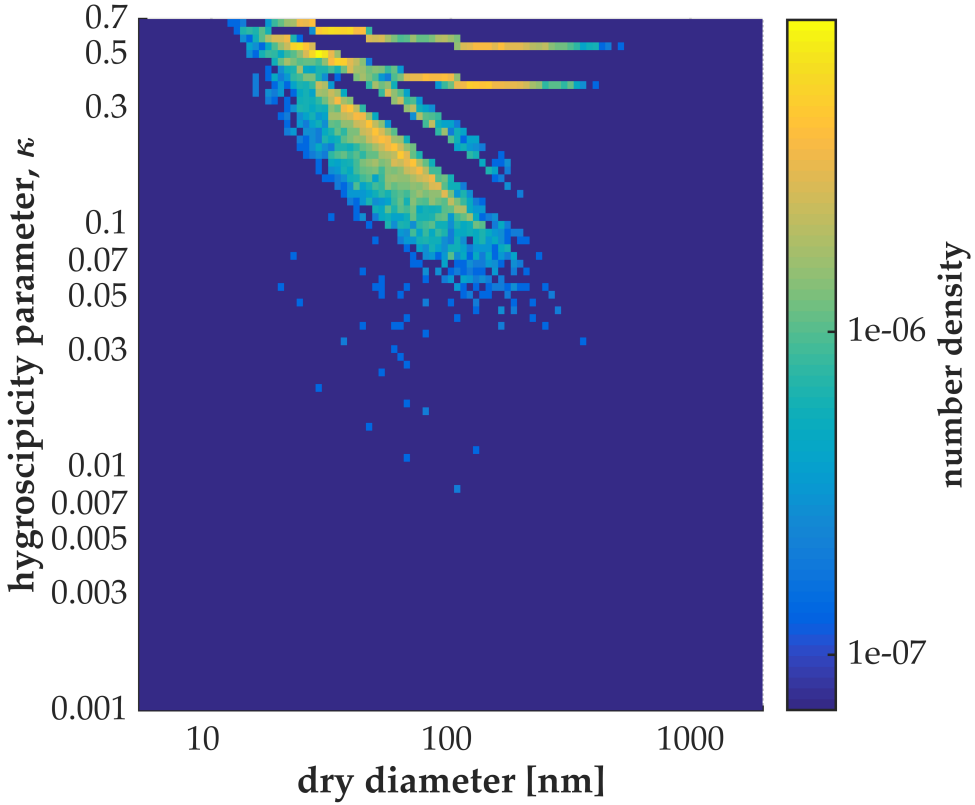
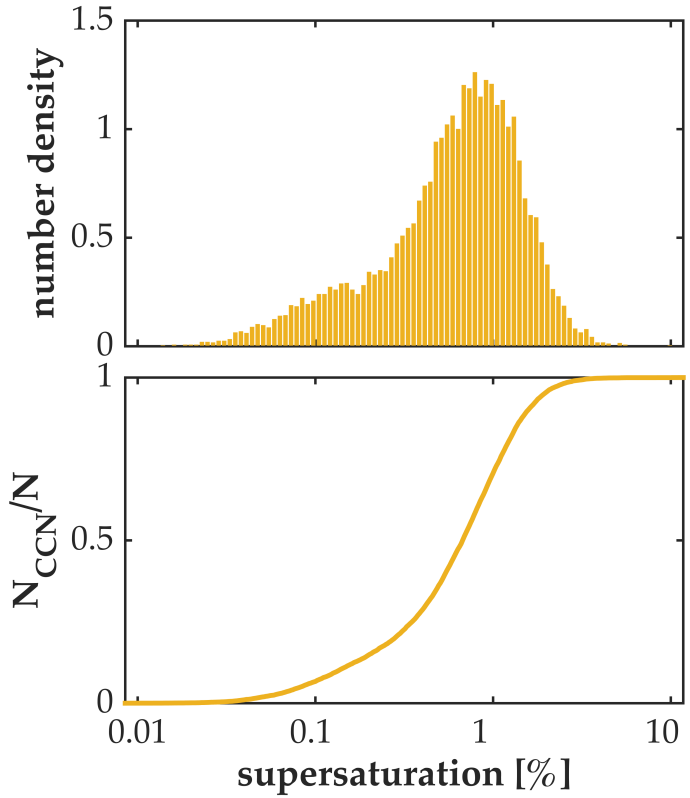
Challenges: Moving beyond box model to integrate quadrature-based model into WRF-Chem for comparison with other schemes evaluation against observations

Planned collaborations: Nicole Riemer and Matt West for benchmarking; Susanne Bauer, Philip Stier, etc. for applying new techniques to advance modal models; and Jerome Fast, etc. for evaluation using the Aerosol Modeling Testbed

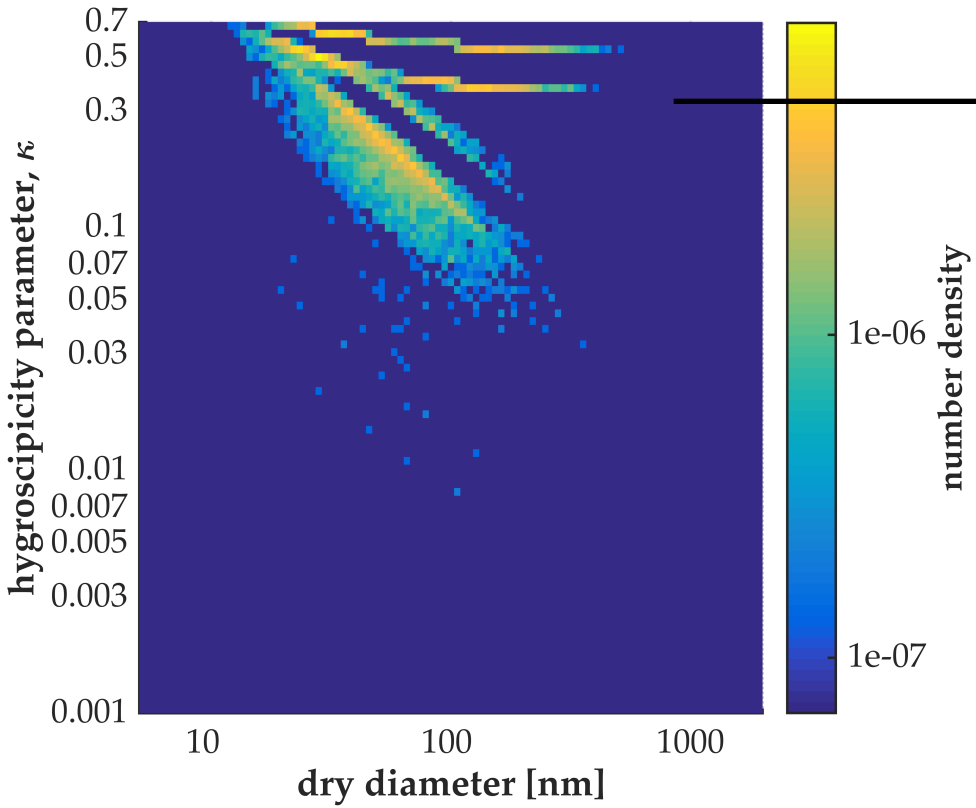
Summary of progress: Demonstrated that sparse quadratures in bivariate coordinates accurately and efficiently describe the CCN spectrum of complex aerosol mixing states for use in models.

Particle-resolved model reveals wide variation in size and κ, leading to variation in CCN activation as a function of *s*.
Can we represent this variability with quadrature-based models?





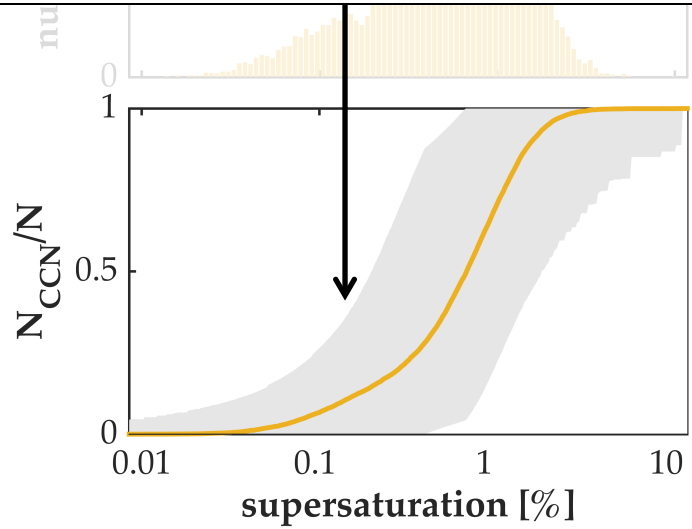
If 7 bivariate moment constraints are known, large uncertainty in in CCN fraction as function of supersaturation



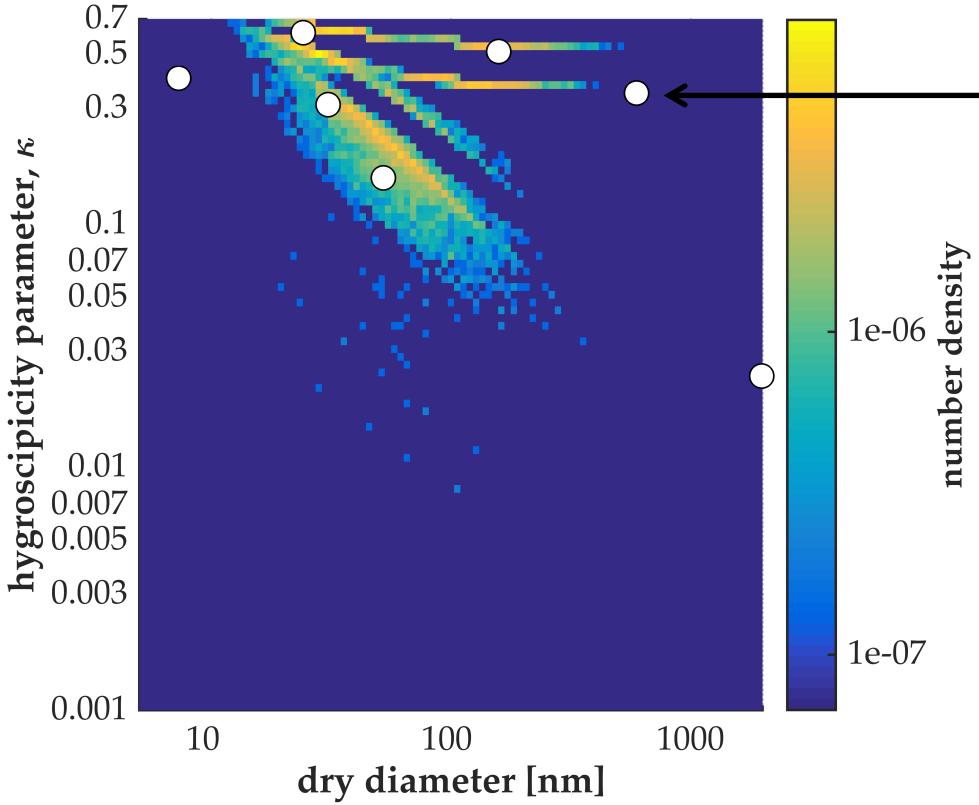
for given bivariate constraints:

$$\mu_k = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} n(D_{\text{dry}},\kappa)\phi_k(D_{\text{dry}},\kappa)dD_{\text{dry}}\,d\kappa,$$

infinite distributions having μ_k set, large span in $N_{\text{CCN}}(s)/N$



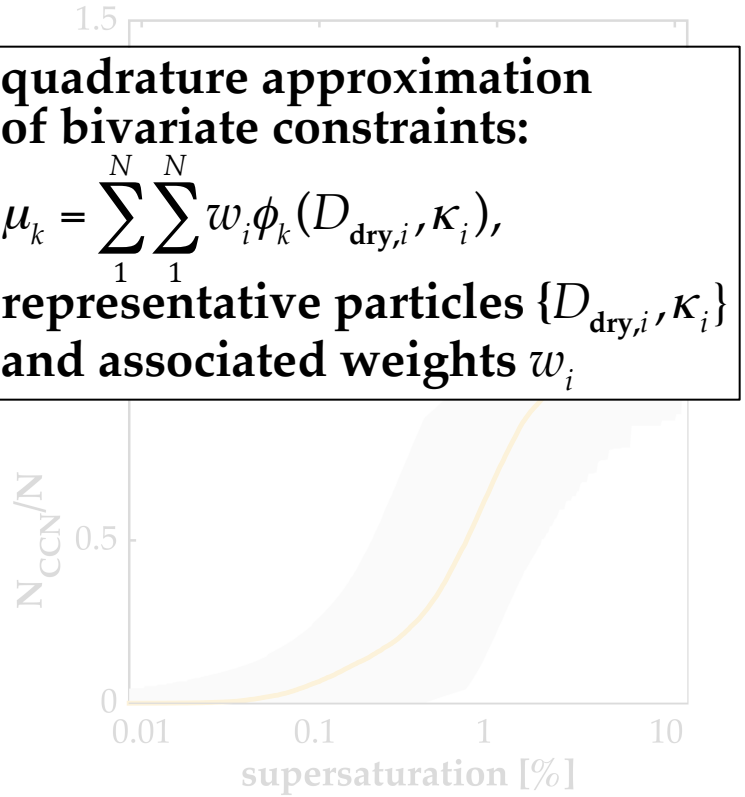
Construct quadrature from bivariate constraints



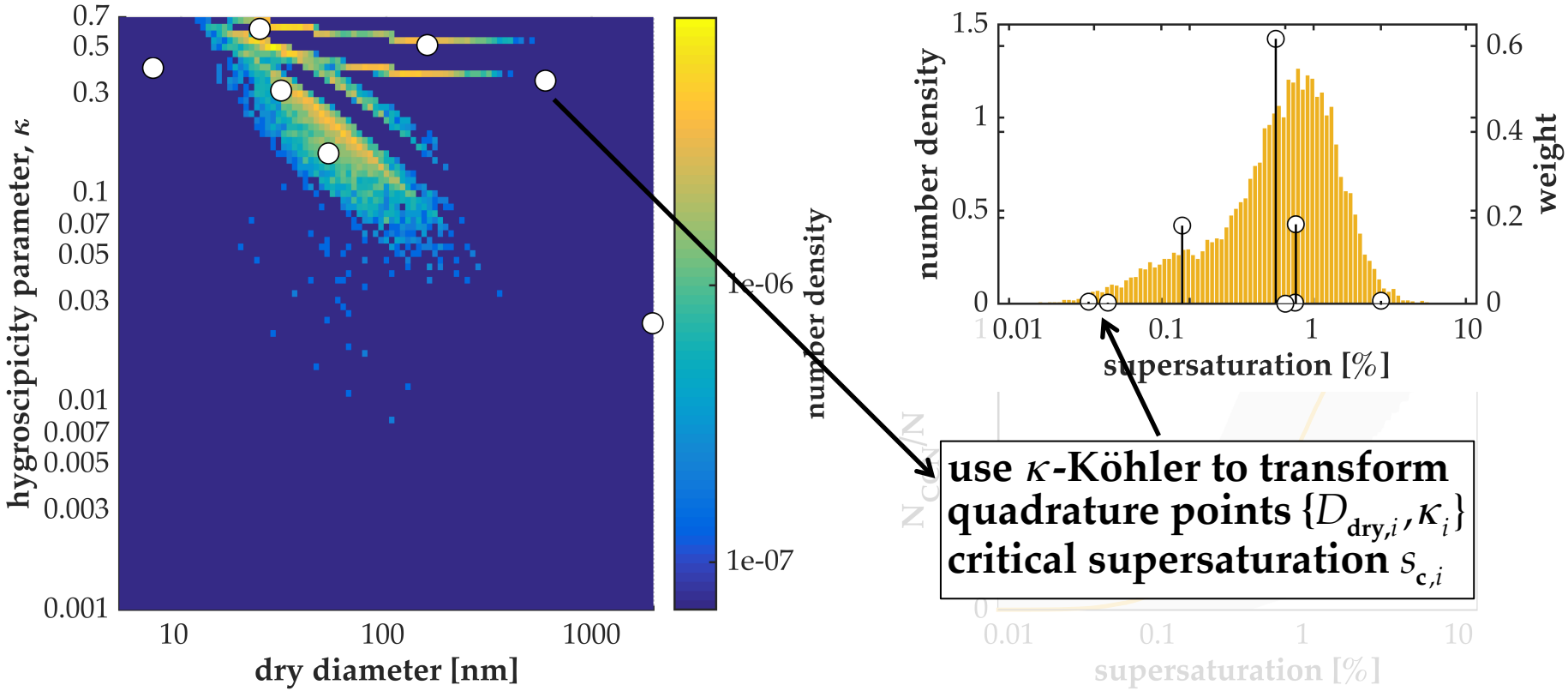
quadrature approximation of bivariate constraints:

$$\mu_k = \sum_{1}^{N}\sum_{1}^{N} w_i \phi_k(D_{\mathrm{dry},i}, \kappa_i),$$

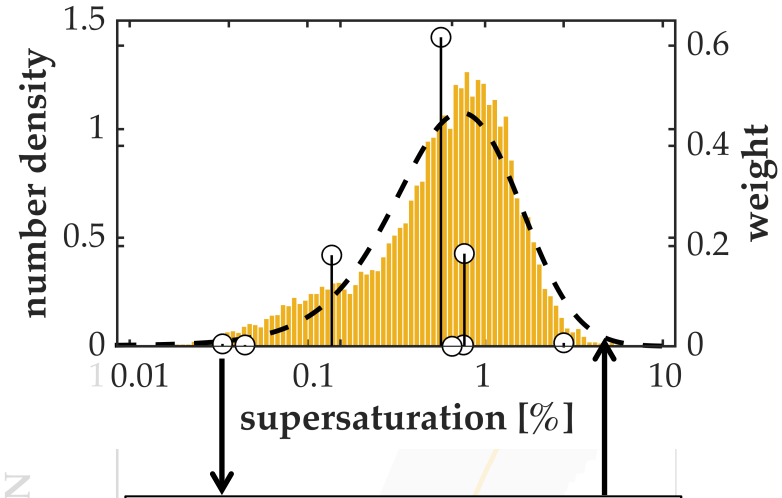
representative particles $\{D_{\mathrm{dry},i}, \kappa_i\}$ **and associated weights** w_i



Compute critical supersaturation $s_{c,i}$ for each sparse particle



Approximately reconstruct number distribution $n(s_c)$ from projected quadrature points $s_{c,i}$ and weights w_i

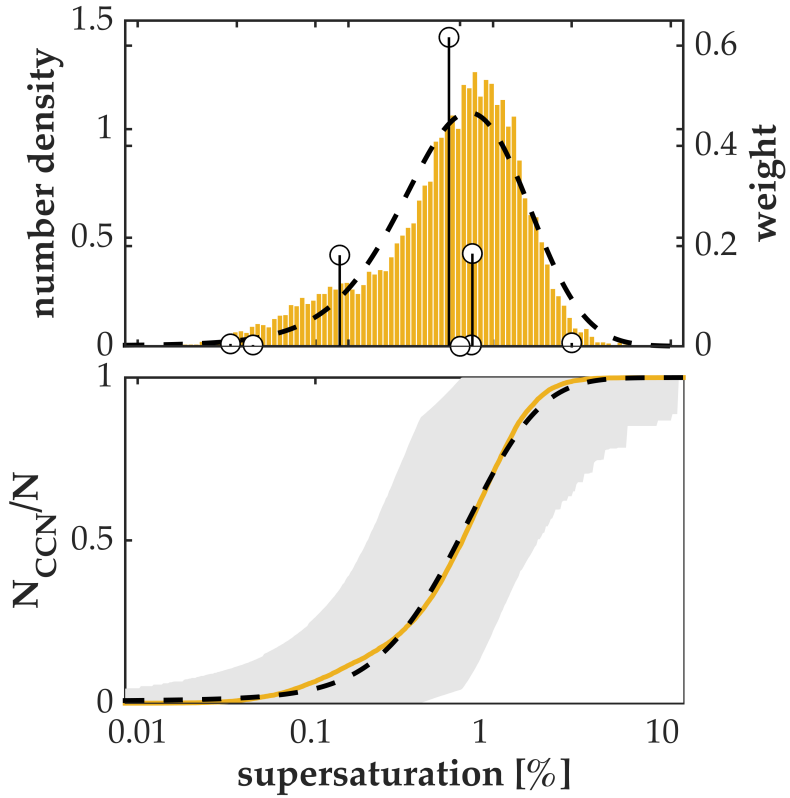


Compute $s_{c,i}$ moments from quadrature points:

$$\mu_n = \sum_1^N w_i \phi_n(s_{c,i}).$$

Reconstruct $n(s_c)$ as constrained maximum entropy distribution.

Quadrature-based reconstruction reproduces CCN spectrum from PartMC-MOSAIC using only 7 sparse particles



Overview of new approach for quadrature-based models

1. simulate few sparse particles

2. project into relevant variable space, e.g. $s_{c,i}$

3. reconstruct number distribution, e.g. $n(s_c)$